NASA IDEAL GAS FORMULATION

Reference document: NASA/TP—2002-211556

NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species

A rich data collection is presented to calculate ideal gas thermodynamic properties.
Specific heat at constant temperature:

$$\frac{C_p^o(T)}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4$$

Enthalpy

$$\frac{H^0(T)}{RT} = -a_1T^{-2} + a_2\frac{ln(T)}{T} + a_3 + a_4\frac{T}{2} + a_5\frac{T^2}{3} + a_6\frac{T^3}{4} + a_7\frac{T^4}{5} + b_1T$$

Entropy

$$\frac{S^0(T)}{R} = -a_1\frac{T^{-2}}{2} - a_2T^{-1} + a_3\ln(T) + a_4T + a_5\frac{T^2}{2} + a_6\frac{T^3}{3} + a_7\frac{T^4}{4} + b_2$$

b1 and b2 is integral constant for the equations. Coefficients are given as table format

$$S(T,P)=S^0(T)-Rln\left(\frac{P}{P_0}\right)$$

Chemical enthalpy: $H_T(T)=H(T)-H(298.15)+\Delta h_f(298.15)$

Chemical entropy : $S_T(T,P) = S(T,P) - S(298.15, P0)$

P0=101.325 kPa

$$G^0(T) = H^0(T) - T * S^0(T)$$

Gibbs energy: $G(T,P)=h(T)-S(T,P)=G^0(T)-RTln\left(\frac{P}{P_0}\right)$

Chemical gibbs energy: $G_T(T,P) = H_T(T) - TS_T(T,P)$

As an alternative equation partial continious curve fitting base Cp equations are used. Partial continues data that is divided into someting like 10 subregion is usually considered more accurate compare to nasa formulation. We will use this set of program development for comparison purposes (Gas_Data and Gas_PG)

$Cp_i(T) = A_i + B_i*10^{-3}*T + C_i*10^5/T^2 + D_i*10^{-6}*T^2$ $\quad T_{Li} >= T > T_{Hi}$ $\quad$ KJ/kmol K

$$h(T) = h_0 + \int_{T_0}^{T_{kN}>T_0} C_{pi}(T)dT + \sum_{k=kN}^{kM}\int_{T_{kN}}^{T_{kM}} C_{pi}(T)dT + \int_{T_{kN}<T}^{T} C_{pi}(T)dT \quad s(T)$$

$$= s_0 + h_0 + \int_{T_0}^{T_{kN}>T_0} \frac{C_{pi}(T)}{T}dT + \sum_{k=kN}^{kM}\int_{T_{kN}}^{T_{kM}} \frac{C_{pi}(T)dT}{T} + \int_{T_{kN}<T}^{T} \frac{C_{pi}(T)}{T}dT - Rln\frac{P}{P_0}$$

Computer programs:

nasa9_Data	Read data from nasa9.txt	
Gas_Data	Partial continious formula	
Gas_PG_nasa9	Nasa based formulation	

Gas_PG	Partial continious based formulation	

Sample outputs:

Results are created by using nasa data and previous ideal gas equation Gas_PG, sample gas is nitrogen (N_2)

Properties of dry air ideal gas EOS based on NASA 9 database

array no	property name	dry air property	unit
0	P, pressure	101.325	kPA
1	T, temperature	273.15	deg K
2	v, specific volume	22.413969545014137	m³/kmol
3	h, enthalpy	0.0	KJ/kmol
4	u, internal energy	0.0	KJ/kmol
5	s, entropy	0.0	KJ/kmolK
6	x, quality	2.0	kg vap/kg mix
7	Cp, specific heat at c...	29.115475799379873	KJ/kmolK
8	Cv, specific heat at c...	20.80101318122663	KJkmolK
9	α isobaric thermal exp...	0.0036609921288669...	1/K
10	κ isothermal compres...	9.86923266716013E-6	1/Pa
11	η Dynamic viscosity	1.662817340802218E-5	Pa.s
12	k Thermal conductivity	0.02576059019220405	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.670881112144658	
15	ρ density	0.044615033405470315	kmol/m³
16	speed of sound	336.8634287484107	m/s

Properties of dry air ideal gas EOS

array no	property name	dry air property	unit
0	P, pressure	101.325	kPA
1	T, temperature	273.15	deg K
2	v, specific volume	22.41396954501...	m³/kmol
3	h, enthalpy	0.0	KJ/kmol
4	u, internal energy	0.0	KJ/kmol
5	s, entropy	0.0	KJ/kmolK
6	x, quality	2.0	kg vap/kg mix
7	Cp, specific heat...	29.11608275854...	KJ/kmolK
8	Cv, specific heat...	20.80162014039...	KJkmolK
9	α isobaric therm...	0.003660992128...	1/K
10	κ isothermal co...	9.869232667160...	1/Pa
11	η Dynamic visco...	1.662817340802...	Pa.s
12	k Thermal condu...	0.025760590192...	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.670906593467...	
15	ρ density	0.044615033405...	kmol/m³
16	speed of sound	336.8649113334...	m/s

Properties of dry air ideal gas EOS based on NASA 9 ...

array no	property name	dry air property	unit
0	P, pressure	101.325	kPA
1	T, temperature	298.15	deg K
2	v, specific volume	24.46540369703...	m³/kmol
3	h, enthalpy	727.9868898633...	KJ/kmol
4	u, internal energy	520.1253244095...	KJ/kmol
5	s, entropy	2.550150627114...	KJ/kmolK
6	x, quality	2.0	kg vap/kg mix
7	Cp, specific heat...	29.12418436007...	KJ/kmolK
8	Cv, specific heat...	20.80972174192...	KJkmolK
9	α isobaric therm...	0.003354016434...	1/K
10	κ isothermal co...	9.869232667160...	1/Pa
11	η Dynamic visco...	1.779177544178...	Pa.s
12	k Thermal condu...	0.027538314695...	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.671689622689...	
15	ρ density	0.040874044523...	kmol/m³
16	speed of sound	351.9206225229...	m/s

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0	P, pressure	101.325	kPA
1	T, temperature	298.15	deg K
2	v, specific volume	24.46540369703...	m³/kmol
3	h, enthalpy	727.9972439591...	KJ/kmol
4	u, internal energy	520.1356785052...	KJ/kmol
5	s, entropy	2.550187271278...	KJ/kmolK
6	x, quality	2.0	kg vap/kg mix
7	Cp, specific heat...	29.12415119712...	KJ/kmolK
8	Cv, specific heat...	20.80968857897...	KJkmolK
9	α isobaric therm...	0.003354016434...	1/K
10	κ isothermal co...	9.869232667160...	1/Pa
11	η Dynamic visco...	1.779177544178...	Pa.s
12	k Thermal condu...	0.027538314695...	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.671700367176...	
15	ρ density	0.040874044523...	kmol/m³
16	speed of sound	351.9237176273...	m/s

Properties of dry air ideal gas EOS based on NASA 9 ...

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5	s, entropy	2.550150627114...	KJ/kmolK
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7	Cp, specific heat...	29.12418436007...	KJ/kmolK
8	Cv, specific heat...	20.80972174192...	KJkmolK
9	α isobaric therm...	0.003354016434...	1/K
10	κ isothermal co...	9.869232667160...	1/Pa
11	η Dynamic visco...	1.779177544178...	Pa.s
12	k Thermal condu...	0.027538314695...	W/mK
13	σ Surface tension	0.0	N/m
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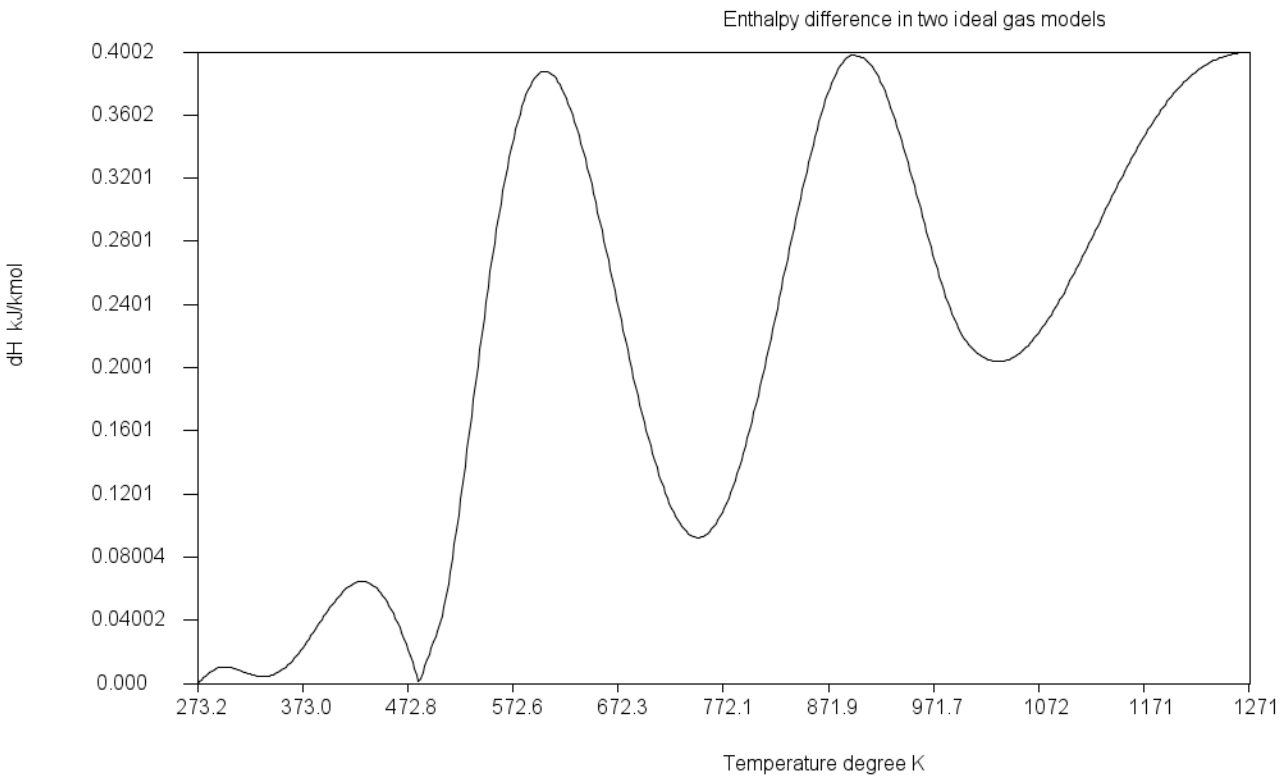
8	Cv, specific heat...	20.80968857897...	KJkmolK
9	α isobaric therm...	0.003354016434...	1/K
10	κ isothermal co...	9.869232667160...	1/Pa
11	η Dynamic visco...	1.779177544178...	Pa.s
12	k Thermal condu...	0.027538314695...	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.671700367176...	
15	ρ density	0.040874044523...	kmol/m³
16	speed of sound	351.9237176273...	m/s

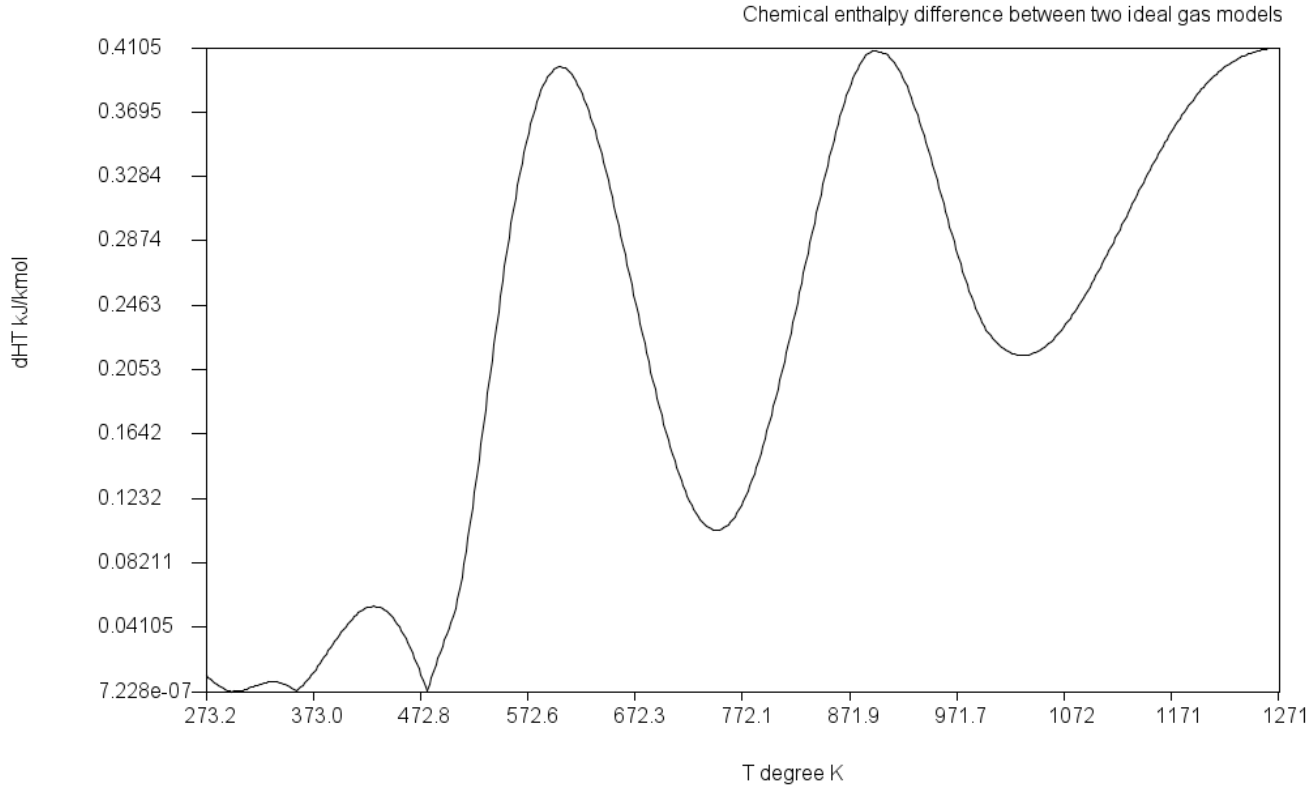
Properties of dry air ideal gas EOS based on NASA 9 database

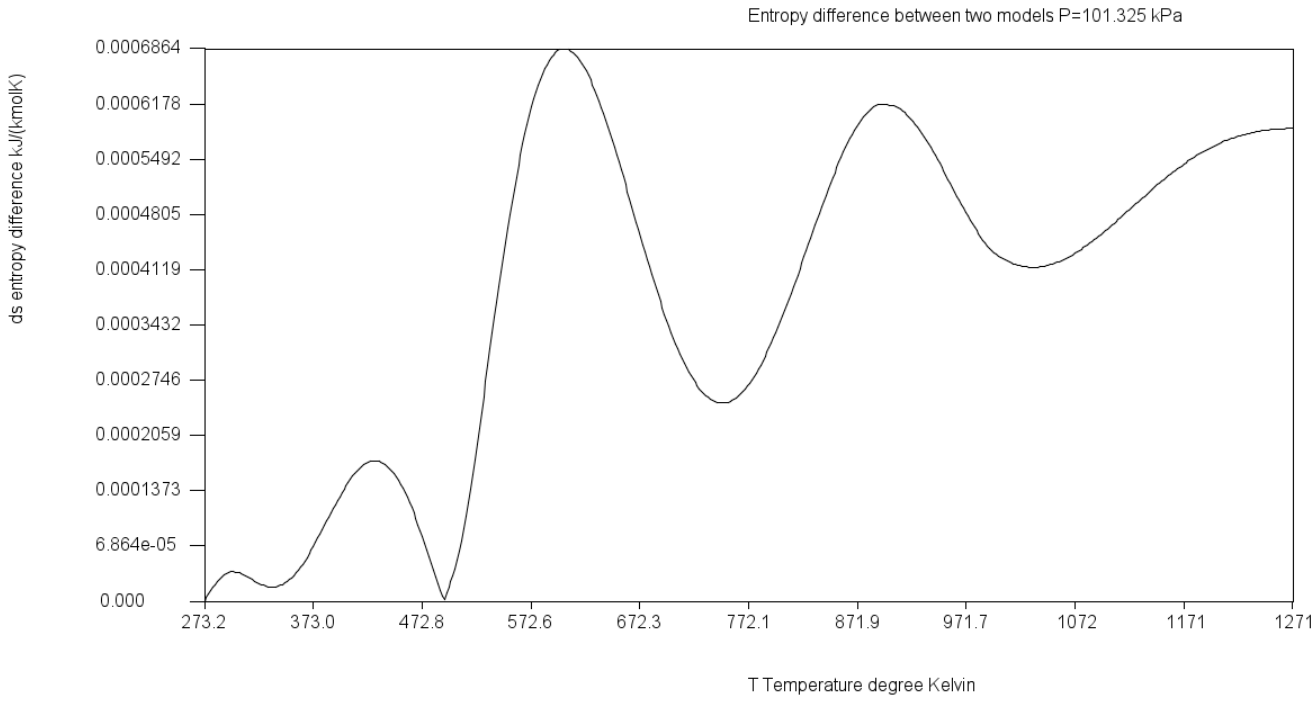
array no	property name	dry air property	unit
0	P, pressure	101.325	kPA
1	T, temperature	473.15	deg K
2	v, specific volume	38.82544276120608	m³/kmol
3	h, enthalpy	5845.990311316274	KJ/kmol
4	u, internal energy	4183.097787685625	KJ/kmol
5	s, entropy	16.05042148657583	KJ/kmolK
6	x, quality	2.0	kg vap/kg mix
7	Cp, specific heat at c...	29.470913629198172	KJ/kmolK
8	Cv, specific heat at c...	21.15645101104493	KJkmolK
9	α isobaric thermal exp...	0.002113494663425975	1/K
10	κ isothermal compres...	9.869232667160127E-6	1/Pa
11	η Dynamic viscosity	2.4843542840457466...	Pa.s
12	k Thermal conductivity	0.03875983628813346	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.6743077198780469	
15	ρ density	0.025756306403263693	kmol/m³
16	speed of sound	442.29127766323506	m/s

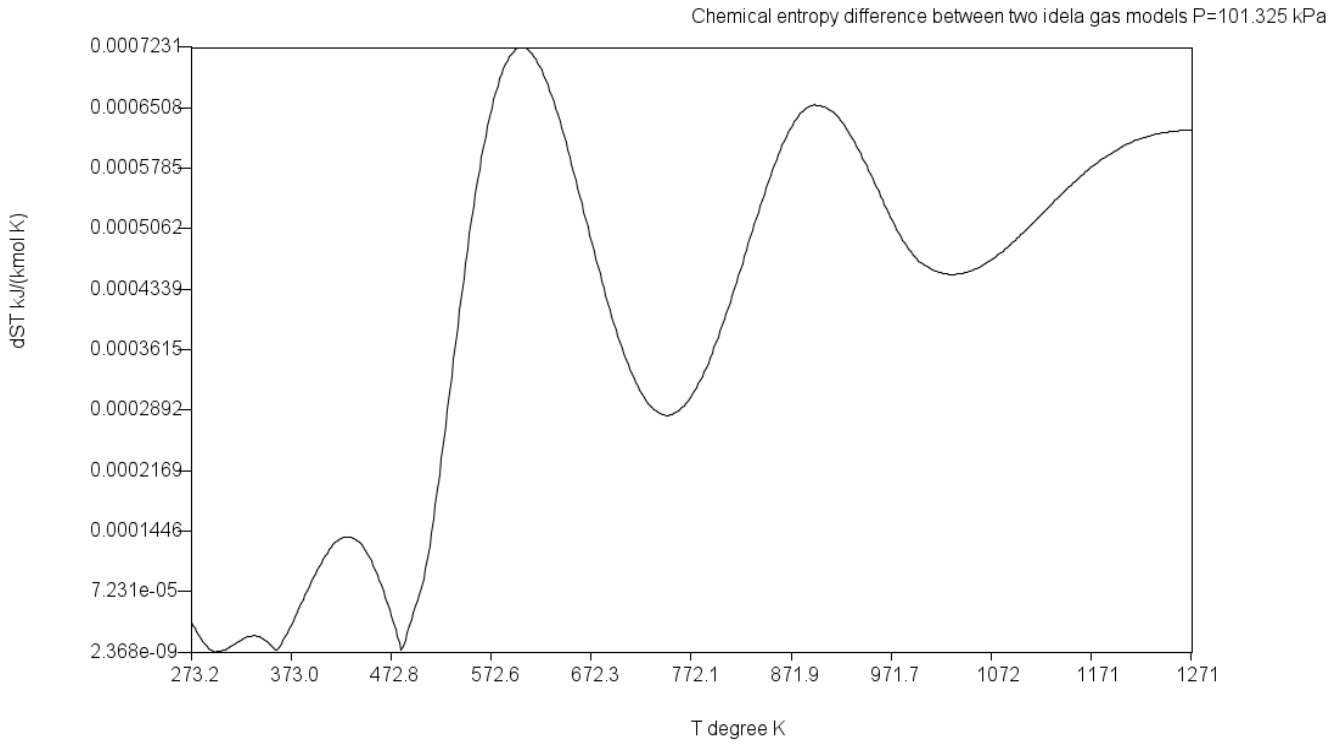
Properties of dry air ideal gas EOS

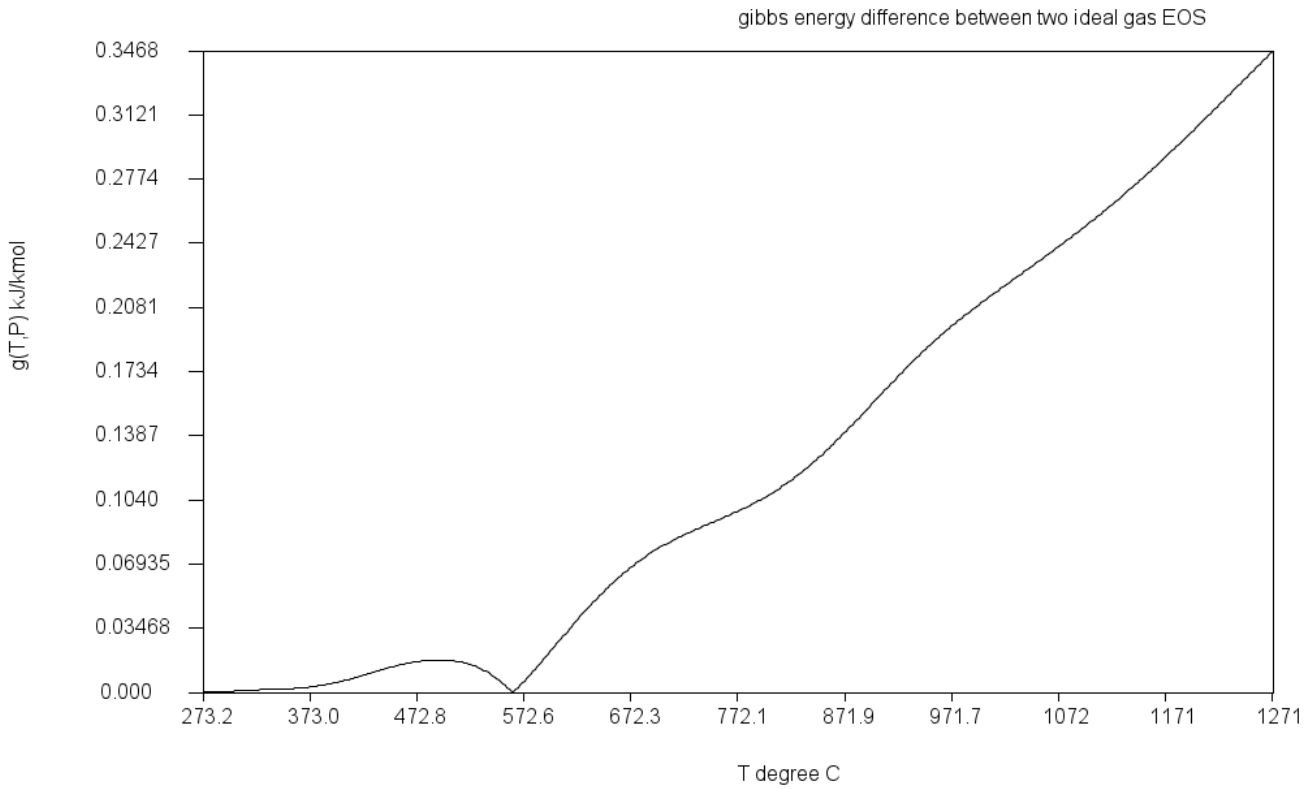
array no	property name	dry air property	unit
0	P, pressure	101.325	kPA
1	T, temperature	473.15	deg K
2	v, specific volume	38.82544276120...	m³/kmol
3	h, enthalpy	5846.011419532...	KJ/kmol
4	u, internal energy	4183.118895901...	KJ/kmol
5	s, entropy	16.05050120825...	KJ/kmolK
6	x, quality	2.0	kg vap/kg mix
7	Cp, specific heat...	29.46905147105...	KJ/kmolK
8	Cv, specific heat...	21.15458885290...	KJkmolK
9	α isobaric therm...	0.002113494663...	1/K
10	κ isothermal co...	9.869232667160...	1/Pa
11	η Dynamic visco...	2.484354284045...	Pa.s
12	k Thermal condu...	0.038759836288...	W/mK
13	σ Surface tension	0.0	N/m
14	Prandtl number	0.674276666331...	
15	ρ density	0.025756306403...	kmol/m³
16	speed of sound	442.3005589738...	m/s

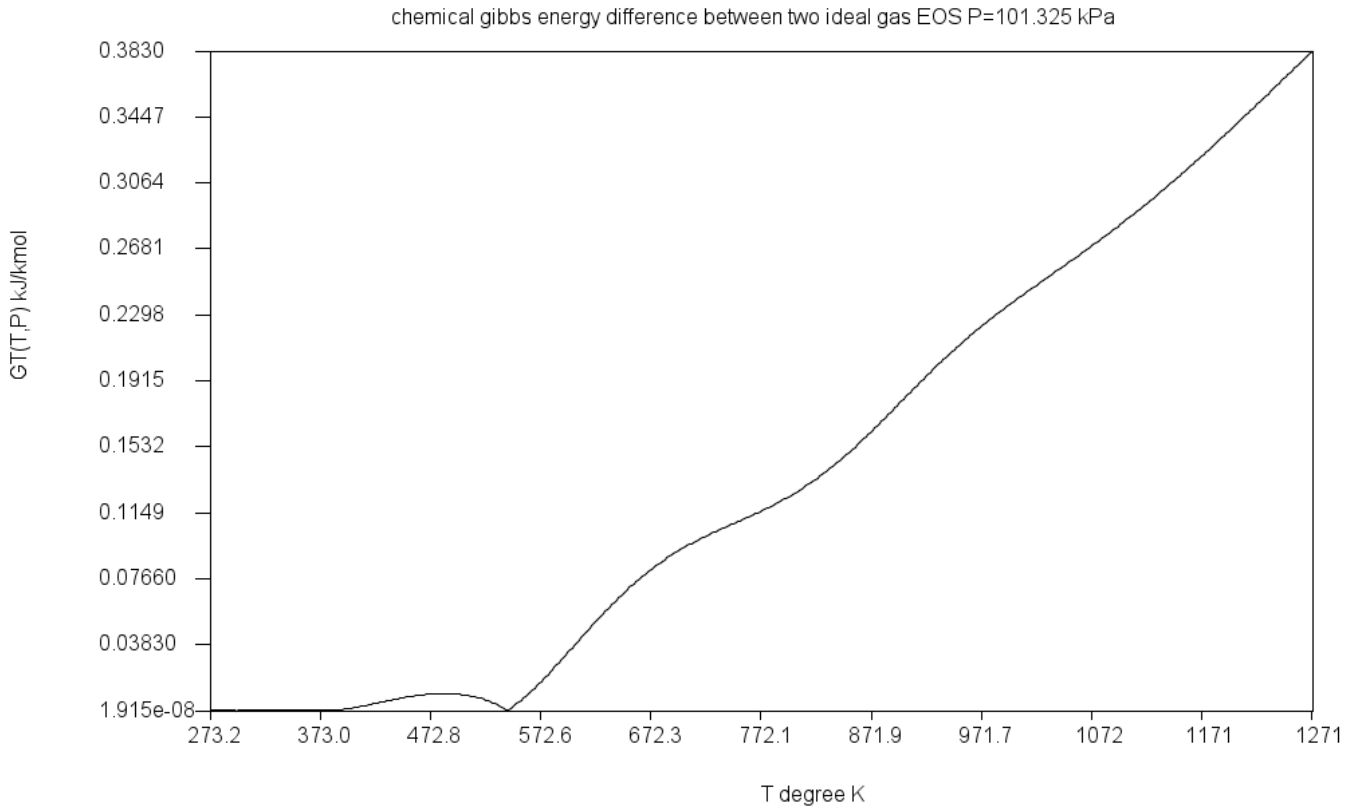



Chemical enthalpy difference between two ideal gas models
dHT kJ/kmol
0.4105
0.3695
0.3284
0.2874
0.2463
0.2053
0.1642
0.1232
0.08211
0.04105
7.228e-07
273.2
373.0
472.8
572.6
672.3
772.1
871.9
971.7
1072
1171
1271
T degree K


Entropy difference between two models P=101.325 kPa
ds entropy difference kJ/(kmolK)
0.0006864
0.0006178
0.0005492
0.0004805
0.0004119
0.0003432
0.0002746
0.0002059
0.0001373
6.864e-05
0.000
273.2
373.0
472.8
572.6
672.3
772.1
871.9
971.7
1072
1171
1271
T Temperature degree Kelvin


Chemical entropy difference between two idela gas models P=101.325 kPa
dST kJ/(kmol K)
0.0007231
0.0006508
0.0005785
0.0005062
0.0004339
0.0003615
0.0002892
0.0002169
0.0001446
7.231e-05
2.368e-09
273.2
373.0
472.8
572.6
672.3
772.1
871.9
971.7
1072
1171
1271
T degree K


gibbs energy difference between two ideal gas EOS
g(T,P) kJ/kmol
0.3468
0.3121
0.2774
0.2427
0.2081
0.1734
0.1387
0.1040
0.06935
0.03468
0.000
273.2
373.0
472.8
572.6
672.3
772.1
871.9
971.7
1072
1171
1271
T degree C



Computer codes:

nasa9_Data

```
import java.io.*;
import java.util.*;
import javax.swing.*;
import javax.swing.table.*;
import java.awt.*;


public class nasa9_Data
{ String name_list[]={"e-","Ag","Ag+","Ag-","AL","AL+","AL-
","ALBO2","ALBr","ALBr2","ALBr3","ALC","ALC2","ALCL","ALCL+","ALCL2","ALCL3","ALCL2+","ALCL2-
","ALF","ALF+","ALFCL","ALFCL+","ALFCL2","ALF2","ALF2+","ALF2-","ALF2CL","ALF3","ALF4-
","ALH","ALHCL","ALHCL2","ALHF","ALHFCL","ALHF2","ALH2","ALH2CL","ALH2F","ALH3","ALI","ALI2","ALI3","ALN","ALO","ALO+","ALO-
","ALOCL","ALOCL2","ALOF","ALOF2","ALOF2-","ALOH","ALOH+","ALOH-","ALOHCL","ALOHCL2","ALOHF","ALOHF2","ALO2","ALO2-
","AL(OH)2","AL(OH)2CL","AL(OH)2F","AL(OH)3","ALS","ALS2","AL2","AL2Br6","AL2C2","AL2CL6","AL2F6","AL2I6","AL2O","AL2O+","AL2O2","AL2O2+","AL2
O3","AL2S","AL2S2","Ar","Ar+","B","B+","B-","BBr","BBr2","BBr3","BC","BC2",
"BCL","BCL+","BCLOH","BCL(OH)2","BCL2","BCL2+","BCL2-","BCL2OH","BCL3","BF","BFCL","BFCL2","BFOH","BF(OH)2","BF2","BF2+","BF2-
","BF2CL","BF2OH","BF3","BF4-","BH","BHCL","BHCL2","BHF","BHFCL","BHF2","BH2","BH2CL","BH2F","BH3","BH3NH3","BI","BI2","BI3","BN","BO","BO-
","BOCL","BOCL2","BOF","BOF2","BOH","BO2","BO2-
","B(OH)2","BS","BS2","B2","B2C","B2CL4","B2F4","B2H6","B2O","B2O2","B2O3","B2(OH)4","B2S","B2S2","B2S3","B3N3H6","B3O3CL3","B3O3FCL2","B3O
3F2CL","B3O3F3","Ba","Ba+","BaBr","BaBr2","BaCL","BaCL+","BaCL2","BaF","BaF+","BaF2","BaH","BaI","BaI2","BaO","BaO+","BaOH","BaOH+","Ba(OH)2","
BaS","Ba2","Be","Be+","Be++","BeBO2","BeBr","BeBr2","BeCL","BeCL+","BeCLF","BeCL2","BeF","BeF2","BeH","BeH+","BeH2","BeI","BeI2","BeN","BeO","B
eOH","BeOH+","Be(OH)2","BeS","Be2","Be2CL4","Be2F4","Be2O","Be2OF2","Be2O2","Be3O3","Be4O4","Br","Br+","Br-
","BrCL","BrF","BrF3","BrF5","BrO","OBrO","BrOO","BrO3","Br2","BrBrO","BrOBr","C","C+","C-
","CBr","CBr2","CBr3","CBr4","CCL","CCLBr3","CCL2","CCL2Br2","CCL3","CCL3Br","CCL4","CF","CF+","CFBr3","CFCL","CFCLBr2","CFCL2","CFCL2Br","CFCL3",
"CF2","CF2+","CF2Br2","CF2CL","CF2CLBr","CF2CL2","CF3","CF3+","CF3Br","CF3CL","CF4","CH","CH+","CHBr3","CHCL","CHCLBr2","CHCL2","CHCL2Br","CHC
L3","CHF","CHFBr2","CHFCL","CHFCLBr","CHFCL2","CHF2","CHF2Br","CHF2CL","CHF3","CH2","CH2Br2","CH2CL","CH2CLBr","CH2CL2","CH2F","CH2FBr","CH
2FCl","CH2F2","CH3","CH3Br","CH3CL","CH3F","CH2OH","CH3O","CH4","CH3OH","Cl","CN","CN+","CN-
","CNN","CO","CO+","COCL","COCL2","COF","COFCL","COF2","COHCL","COHF","COS","CO2","CO2+","COOH","CP","CS","CS2","C2","C2+","C2-
","C2CL","C2CL2","C2CL3","C2CL4","C2CL6","C2F","C2FCL","C2FCL3","C2F2","C2F2CL2","C2F3","C2F3CL","C2F4","C2F6","C2H","C2HCL","C2HCL3","C2HF","
C2HFCL2","C2HF2CL","C2HF3","CHCO,ketyl","C2H2,vinylidene","C2H2,acetylene","C2H2CL2","C2H2FCL","C2H2F2","CH2CO,ketene","C2H3,vinyl","C2H3CL",
"C2H3F","CH3CN","CH3CO,acetyl","C2H4","C2H4O,ethylen-
o","CH3CHO,ethanal","CH3COOH","C2H5","C2H5Br","C2H6","CH3N2CH3","C2H5OH","CH3OCH3","CCN","CNC","C2N2","C2O","C3","C3H3,1-
propynl","C3H3,2-propynl","C3H4,allene","C3H4,propyne","C3H4,cyclo-","C3H5,allyl","C3H6,propylene","C3H6,cyclo-","C3H6O","C3H7,n-propyl","C3H7,i-
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propyl","C3H8","C3H8O,1propanol","C3H8O,2propanol","C3O2","C4","C4H2","C4H4,1,3-cyclo-","C4H6,butadiene","C4H6,1-butyne","C4H6,2-
butyne","C4H6,cyclo-","C4H8,1-butene","C4H8,cis2-buten","C4H8,tr2-butene","C4H8,isobutene","C4H8,cyclo-","(CH3COOH)2","C4H9,n-butyl","C4H9,i-
butyl","C4H9,s-butyl","C4H9,t-butyl","C4H10,isobutane","C4H10,n-butane","C4N2","C5","C5H6,1,3cyclo-","C5H8,cyclo-","C5H10,1-pentene","C5H10,cyclo-
","C5H11,pentyl","C5H11,t-pentyl","C5H12,n-pentane","C5H12,i-
pentane","CH3C(CH3)2CH3","C6H2","C6H5,phenyl","C6D5,phenyl","C6H5O,phenoxy","C6H6","C6D6","C6H5OH,phenol","C6H10,cyclo-","C6H12,1-
hexene","C6H12,cyclo-","C6H13,n-hexyl","C6H14,n-hexane","C7H7,benzyl","C7H8","C7H8O,cresol-mx","C7H14,1-heptene","C7H15,n-heptyl","C7H16,2-
methylh","C7H16,n-heptane","C8H8,styrene","C8H10,ethylbenz","C8H16,1-octene","C8H17,n-octyl","C8H18,n-octane","C8H18,isooctane","C9H19,n-
nonyl","C10H8,naphthale","C10H21,n-decyl","C12H9,o-bipheny","C12D9,o-
bipheny","C12H10,biphenyl","C12D10,biphenyl","Ca","Ca+","CaBr","CaBr2","CaCL","CaCL+","CaCL2","CaF","CaF+","CaF2","CaH","CaI","CaI2","CaO","CaO+"
,"CaOH","CaOH+","Ca(OH)2","CaS","Ca2","Cd","Cd+","CL","CL+","CL-","CLCN","CLF","CLF3","CLF5","CLO","CLO2","CL2","CL2O","Co","Co+","Co-
","Cr","Cr+","Cr-","CrN","CrO","CrO2","CrO3","Cs","Cs+","Cs-
","CsCL","CsF","CsO","CsOH","CsOH+","Cs2","Cs2CL2","Cs2F2","Cs2O","Cs2O2H2","Cs2SO4","Cu","Cu+","Cu-
","CuCL","CuF","CuF2","CuO","Cu2","Cu3CL3","D","D+","D-","DBr","DCL","DF","DOCL","DO2","DO2-","D2","D2+","D2-","D2O","D2O2","D2S","F","F+","F-
","FCN","FO","FO2,FOO","FO2,OFO","F2","F2O","F2O2","FS2F,fluorodisu","Fe","Fe+","Fe-
","FeC5O5","FeCL","FeCL2","FeCL3","FeO","Fe(OH)2","Fe2CL4","Fe2CL6","GaBr","GaBr2","GaBr3","GaCL","GaCL2","GaCL3","GaF","GaF2","GaF3","GaH","G
aI","GaI2","GaI3","GaO","GaOH","Ga2Br2","Ga2Br4","Ga2Br6","Ga2CL2","Ga2CL4","Ga2CL6","Ga2F2","Ga2F4","Ga2F6","Ga2I2","Ga2I4","Ga2I6","Ga2O","
Ge","Ge+","Ge-",
"GeBr","GeBr2","GeBr3","GeBr4","GeCL","GeCL2","GeCL3","GeCL4","GeF","GeF2","GeF3","GeF4","GeI","GeO","GeO2","GeS","GeS2","Ge2","H","H+","H-
","HALO","HALO2","HBO","HBO+","HBO-","HBO2","HBS","HBS+","HBr","HCN","HCO","HCO+","HCCN","HCL","HD","HD+","HD-
","HDO","HDO2","HDO2","HF","HI","HNC","HNCO","HNO","HNO2","HNO3","HOCL","HOF","HO2","HO2-","HPO","HSO3F","H2","H2+","H2-
","HBOH","HCHO,formaldehy","HCOOH","H2F2","H2O","H2O+","H2O2","H2S","H2SO4","H2BOH","HB(OH)2","H3BO3","H3B3O3","H3B3O6","H3F3","H3O+
","(HCOOH)2","H4F4","H5F5","H6F6","H7F7","He","He+","Hg","Hg+","HgBr2","I","I+","I-
","IF5","IF7","I2","In","In+","InBr","InBr2","InBr3","InCL","InCL2","InCL3","InF","InF2","InF3","InH","InI","InI2","InI3","InO","InOH","In2Br2","In2Br4","In2Br
6","In2CL2","In2CL4","In2CL6","In2F2","In2F4","In2F6","In2I2","In2I4","In2I6","In2O","K","K+","K-","KBO2","KCN","KCL","KF","KF2-","KH","KO","KO-
","KOH","KOH+","K2","K2C2N2","K2CL2","K2F2","K2O2H2","K2SO4","Kr","Kr+","Li","Li+","Li-","LiALF4","LiBO2","LiCL","LiF","LiFO","LiF2-
","LiH","LiN","LiO","LiO-
","LiOH","LiOH+","LiON","Li2","Li2CL2","Li2F2","Li2O","Li2O2","Li2O2H2","Li2SO4","Li3CL3","Li3F3","Mg","Mg+","MgBr","MgBr2","MgCL","MgCL+","MgCLF
","MgCL2","MgF","MgF+","MgF2","MgF2+","MgH","MgI","MgI2","MgN","MgO","MgOH","MgOH+","Mg(OH)2","MgS","Mg2","Mg2F4","Mn","Mn+","Mo","
Mo+","Mo-","MoO3","Mo2O6","Mo3O9","Mo4O12","Mo5O15","N","N+","N-
","NCO","ND","ND2","ND3","NF","NF2","NF3","NH","NH+","NHF","NHF2","NH2","NH2F","NH3","NH4+","NO","NO+","NOCL","NOF","NOF3","NO2","NO2-
","NO2CL","NO2F","NO3","NO3-","NO3F","N2","N2+","N2-","NCN","cis-
N2D2","N2F2","N2F4","N2H2","NH2NO2","N2H4","N2O","N2O+","N2O3","N2O4","N2O5","N3","N3H","Na","Na+","Na-
","NaALF4","NaBO2","NaBr","NaCN","NaCL","NaF","NaF2-","NaH","NaI","NaO","NaO-
","NaOH","NaOH+","Na2","Na2C2N2","Na2CL2","Na2F2","Na2O","Na2O2H2","Na2SO4","Nb","Nb+","Nb-
","NbCL5","NbO","NbOCL3","NbO2","Ne","Ne+","Ni","Ni+","Ni-","NiCL","NiCL2","NiO","NiS","O","O+","O-","OD","OD-","OH","OH+","OH-","O2","O2+","O2-
","O3","P","P+","P-","PCL","PCL2","PCL2-","PCL3","PCL5","PF","PF+","PF-","PFCL","PFCL-","PFCL2","PFCL-","PFCL4","PF2","PF2-
","PF2CL","PF2CL3","PF3","PF3CL2","PF4CL","PF5","PH","PH2","PH2-","PH3","PN","PO","PO-","POCL3","POFCL2","POF2CL","POF3","PO2","PO2-
","PS","P2","P2O3","P2O4","P2O5","P3","P3O6","P4","P4O6","P4O7","P4O8","P4O9","P4O10","Pb","Pb+","Pb-
","PbBr","PbBr2","PbBr3","PbBr4","PbCL","PbCL+","PbCL2","PbCL2+","PbCL3","PbCL4","PbF","PbF2","PbF3","PbF4","PbI","PbI2","PbI3","PbI4","PbO","PbO
2","PbS","PbS2","Pb2","Rb","Rb+","Rb-","RbOH","Rb2O2H2","Rn","Rn+","S","S+","S-","SCL","SCL2","SCL2+","SD","SF","SF+","SF-","SF2","SF2+","SF2-
","SF3","SF3+","SF3-","SF4","SF4+","SF4-","SF5","SF5+","SF5-","SF6","SF6-","SH","SH-","SN","SO","SO-","SOF2","SO2","SO2-
","SO2CLF","SO2CL2","SO2F2","SO3","S2","S2-","S2CL2","S2F2,thiothony","S2O","S3","S4","S5","S6","S7","S8","Sc","Sc+","Sc-","Si","Si+","Si-
","SiBr","SiBr2","SiBr3","SiBr4","SiC","SiC2","SiC4H12","SiCL","SiCL2","SiCL3","SiCL4","SiF","SiFCL","SiF2","SiF3","SiF4","SiH","SiH+","SiHBr3","SiHCL","SiHCL
3","SiHF","SiHF3","SiHI3","SiH2","SiH2Br2","SiH2CL2","SiH2F2","SiH2I2","SiH3","SiH3Br","SiH3CL","SiH3F","SiH3I","SiH4","SiI","SiI2","SiN","SiO","SiO2","SiS
","SiS2","Si2","Si2C","Si2N","Si3","Sn","Sn+","Sn-
","SnBr","SnBr2","SnBr3","SnBr4","SnCL","SnCL2","SnCL3","SnCL4","SnF","SnF2","SnF3","SnF4","SnI","SnI2","SnI3","SnI4","SnO","SnO2","SnS","SnS2","Sn2"
,"Sr","Sr+","SrBr","SrBr2","SrCL","SrCL+","SrCL2","SrF","SrF+","SrF2","SrH","SrI","SrI2","SrO","SrO+","SrOH","SrOH+","Sr(OH)2","SrS","Sr2","Ta","Ta+","Ta-
","TaCL5","TaO","TaO2","Ti","Ti+","Ti-","TiCL","TiCL2","TiCL3","TiCL4","TiO","TiOCL","TiOCL2","TiO2","V","V+","V-","VCL4","VN","VO","VO2","W","W+","W-
","WCL6","WOCL4","WO2","WO2CL2","WO3","WO3-","(WO3)2","(WO3)3","(WO3)4","(WO3)5","Xe","Xe+","Zn","Zn+","Zr","Zr+","Zr-
","ZrN","ZrO","ZrO+","ZrO2","Ag(cr)","Ag(L)","AL(cr)","AL(L)","ALBr3(cr)","ALBr3(L)","ALCL3(cr)","ALCL3(L)","ALF3(II)","ALF3(I)","ALH3(a)","ALI3(cr)","ALI3(L)
","ALN(cr)","ALN(L)","AL(OH)3(a)","AL2O3(a)","AL2O3(L)","AL2S3(a)","AL2S3(b)","AL2S3(L)","AL2SiO5(an)","AL4C3(cr)",
"AL6Si2O13(s)","B(b)","B(L)","BN(cr)","BN(L)","B2O3(cr)","B2O3(L)","B2S3(cr)","B2S3(L)","B3O3H3(cr)","B4C(cr)","B4C(cr)","Ba(cr)","Ba(L)","BaBr2(cr)","Ba
Br2(L)","BaCO3(a)","BaCO3(b)","BaCO3(c)","BaCO3(L)","BaCL2(a)","BaCL2(b)","BaCL2(L)","BaF2(a)","BaF2(b)","BaF2(c)","BaF2(L)","BaI2(cr)","BaI2(L)","BaH
2(a)","BaH2(b)","BaH2(L)","BaO(cr)","BaO(L)","Ba(OH)2(b)","Ba(OH)2(a)","Ba(OH)2(L)","BaS(cr)","BaS(L)","BaSO4(a)","BaSO4(b)","BaSO4(L)","Be(a)","Be(b)
","Be(L)","BeAL2O4(s)","BeAL2O4(L)","BeBr2(cr)","BeBr2(L)","BeCO3(cr)","BeCL2(a)","BeCL2(b)","BeCL2(L)","BeF2(a)","BeF2(b)","BeF2(L)","BeI2(cr)","BeI2(
L)","BeO(a)","BeO(b)","BeO(L)","Be(OH)2(b)","BeS(cr)","BeSO4(a)","BeSO4(b)","BeSO4(c)","BeSO4(L)","Be2C(s)","Be2C(L)","Be3N2(a)","Be3N2(b)","Be3N2(
L)","Br2(cr)","Br2(L)","C(gr)","Ca(a)","Ca(b)","Ca(L)","CaBr2(cr)","CaBr2(L)","CaCO3(cr)","CaCO3(L)","CaCL2(cr)","CaCL2(L)","CaF2(a)","CaF2(b)","CaF2(L)","C
aH2(a)","CaH2(b)","CaH2(L)","CaI2(cr)","CaI2(L)","CaO(cr)","CaO(L)","Ca(OH)2(cr)","Ca(OH)2(L)","CaS(cr)","CaS(L)","CaSO4(II)","CaSO4(I)","CaSO4(L)","Cd(cr
)","Cd(L)","Co(a)","Co(b)","Co(b)","Co(L)","Cr(cr)","Cr(cr)","Cr(cr)","Cr(L)","CrN(s)","Cr2N(s)","Cr2O3(s)","Cr2O3(L)","Cs(cr)","Cs(L)","CsCL(a)","CsCL(b)","CsC
L(L)","CsF(s)","CsF(L)","CsOH(b)","CsOH(c)","CsOH(L)","Cs2SO4(II)","Cs2SO4(I)","Cs2SO4(L)","Cu(cr)","Cu(L)","CuF(s)","CuF2(s)","CuF2(L)","CuO(s)","CuO2H2
(s)","CuSO4(s)","Cu2O(s)","Cu2O(L)","Cu2O5S(s)","Fe(a)","Fe(a)","Fe(c)","Fe(d)","Fe(L)","FeC5O5(L)","FeCL2(s)","FeCL2(L)","FeCL3(s)","FeCL3(L)","FeO(s)","
FeO(L)","Fe(OH)2(s)","Fe(OH)3(s)","FeS(a)","FeS(b)","FeS(c)","FeS(L)","FeSO4(s)","FeS2(s)","Fe2O3(s)","Fe2S3O12(s)","Fe3O4(s)","Ga(cr)","Ga(L)","GaBr3(cr
)","GaBr3(L)","GaCL3(cr)","GaCL3(L)","GaF3(cr)","GaI3(cr)","GaI3(L)","Ga2O3(cr)","Ga2O3(L)","Ge(cr)","Ge(L)","GeO2(II)","GeO2(I)","GeO2(L)","GeS(cr)","G
eS(L)","GeS2(cr)","GeS2(L)","HBO2(cr)","HBO2(L)","H2O(s)","H2O(L)","H2SO4(L)","H3BO3(cr)","H3BO3(L)","H3PO4(cr)","H3PO4(L)","Hg(cr)","Hg(L)","HgBr2
(s)","HgBr2(L)","HgO(s)","I2(cr)","I2(L)","In(cr)","In(L)","InBr(cr)","InBr(L)","InBr3(cr)","InBr3(L)","InCL(crII)","InCL(crI)","InCL(L)","InCl3(cr)","InCl3(L)","InF3(c
r)","InF3(L)","InI(cr)","InI(L)","InI2(crII)","InI2(crI)","InI2(L)","InI3(cr)","InI3(L)","In2O3(cr)","In2O3(L)","K(cr)","K(L)","KCN(s)","KCN(L)","KCL(s)","KCL(L)","KF(s
)","KF(L)","KHF2(a)","KHF2(b)","KHF2(L)","KOH(a)","KOH(b)","KOH(c)","KOH(L)","KO2(s)","K2CO3(s)","K2CO3(L)","K2O(s)","K2O2(s)","K2S(1)","K2S(2)","K2S(
3)","K2S(L)","K2SO4(a)","K2SO4(b)","K2SO4(L)","Li(cr)","Li(L)","LiALO2(s)","LiALO2(L)","LiCL(s)","LiCL(L)","LiF(s)","LiF(L)","LiH(s)","LiH(L)","LiOH(cr)","LiOH(L)
","Li2O(s)","Li2O(L)","Li2SO4(a)","Li2SO4(b)","Li2SO4(L)","Li3N(s)","Mg(cr)","Mg(L)","MgAL2O4(s)","MgAL2O4(L)","MgBr2(cr)","MgBr2(L)","MgCO3(cr)","M
gCO3(L)","MgCL2(cr)","MgCL2(L)","MgF2(cr)","MgF2(L)","MgH2(b)","MgH2(L)","MgI2(cr)","MgI2(L)","MgO(cr)","MgO(L)","Mg(OH)2(cr)","Mg(OH)2(L)","Mg
S(cr)","MgS(L)","MgSO4(II)","MgSO4(I)","MgSO4(L)","MgSiO3(I)","MgSiO3(II)","MgSiO3(III)","MgSiO3(L)","MgTiO3(s)","MgTiO3(L)","MgTi2O5(s)","MgTi2O5

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(L)","Mg2SiO4(s)","Mg2SiO4(L)","Mg2TiO4(s)","Mg2TiO4(L)","Mg3N2(cr)","Mn(a)","Mn(b)","Mn(c)","Mn(d)","Mn(L)","Mo(cr)","Mo(L)","NH4CL(a)","NH4CL
(b)","NH4F(cr)","NH4F(L)","Na(cr)","Na(L)","NaALO2(a)","NaALO2(b)","NaBr(s)","NaBr(L)","NaCN(s)","NaCN(L)","NaCL(s)","NaCL(L)","NaF(s)","NaF(L)","NaI(
s)","NaI(L)","NaOH(a)","NaOH(b)","NaOH(c)","NaOH(L)","NaO2(s)","Na2CO3(I)","Na2CO3(II)","Na2CO3(L)","Na2O(c)","Na2O(a)","Na2O(L)","Na2O2(a)","Na
2O2(b)","Na2S(1)","Na2S(2)","Na2S(L)","Na2SO3(s)","Na2SO3(L)","Na2SO4(V)","Na2SO4(IV)","Na2SO4(I)","Na2SO4(L)","Na3ALF6(a)","Na3ALF6(b)","Na3AL
F6(L)","Na5AL3F14(s)","Na5AL3F14(L)","Nb(cr)","Nb(L)","NbO(s)","NbO(L)","NbOCL3(cr)","NbO2(I)","NbO2(II)","NbO2(III)","NbO2(L)","Nb2O5(s)","Nb2O5(L
)","Ni(cr)","Ni(cr)","Ni(L)","NiS(b)","NiS(a)","NiS(L)","NiS2(s)","NiS2(L)","Ni3S2(I)","Ni3S2(II)","Ni3S2(L)","Ni3S4(s)","P(cr)","P(L)","P4O10(cr)","P4O10(L)","Pb
(cr)","Pb(L)","PbBr2(s)","PbBr2(L)","PbCL2(cr)","PbCL2(L)","PbF2(II)","PbF2(I)","PbF2(L)","PbI2(s)","PbI2(L)","PbO(II-r)","PbO(I-y)","PbO(L)","PbO2(s)",
"PbS(cr)","PbS(L)","Pb2O3(s)","Pb3O4(cr)","Rb(cr)","Rb(L)","RbOH(b)","RbOH(c)","RbOH(L)","S(cr1)","S(cr2)","S(L)","SCL2(L)","S2CL2(L)","Sc(a)","Sc(b)","Sc(l
)","Si(cr)","Si(L)","SiC(b)","SiC(b)","SiC(L)","SiO2(a-qz)","SiO2(b-qz)","SiO2(b-
crt)","SiO2(L)","SiS(cr)","SiS(L)","SiS2(cr)","SiS2(L)","Si2N2O(s)","Si3N4(cr)","Sn(cr)","Sn(L)","SnBr2(cr)","SnBr2(L)","SnBr4(cr)","SnBr4(L)","SnCL2(cr)","SnCL2
(L)","SnCL4(L)","SnF2(cr)","SnF2(L)","SnI2(cr)","SnI2(L)","SnI4(cr)","SnI4(L)","SnO(cr)","SnO(L)","SnO2(cr)","SnO2(L)","SnS(rh)","SnS(cu)","SnS(L)","SnS2(cr)",
"Sr(a)","Sr(b)","Sr(L)","SrBr2(a)","SrBr2(b)","SrBr2(L)","SrCO3(a)","SrCO3(b)","SrCO3(c)","SrCO3(L)","SrCL2(a)","SrCL2(b)","SrCL2(L)","SrF2(a)","SrF2(b)","SrF
2(L)","SrH2(a)","SrH2(b)","SrH2(L)","SrI2(cr)","SrI2(L)","SrO(cr)","SrO(L)","Sr(OH)2(b)","Sr(OH)2(a)","Sr(OH)2(L)","SrS(cr)","SrS(L)","SrS04(a)","SrS04(b)","SrS
04(L)","Ta(cr)","Ta(L)","TaC(s)","TaC(L)","Ta2O5(s)","Ta2O5(L)","Th(a)","Th(b)","Th(L)","Ti(a)","Ti(b)","Ti(L)","TiB(cr)","TiB2(cr)","TiB2(L)","TiC(s)","TiC(L)","Ti
CL2(s)","TiCL3(s)","TiCL4(L)","TiN(s)","TiN(L)","TiO(a)","TiO(b)","TiO(L)","TiO2(ru)","TiO2(L)","Ti2O3(a)","Ti2O3(b)","Ti2O3(L)","Ti3O5(a)","Ti3O5(b)","Ti3O5(
L)","Ti4O7(s)","Ti4O7(L)","U(a)","U(b)","U(c)","U(L)","V(cr)","V(L)","VCL2(s)","VCL3(s)","VCL4(L)","VN(s)","VO(s)","VO(L)","V2O3(s)","V2O3(L)","V2O4(I)","V
2O4(II)","V2O4(L)","V2O5(s)","V2O5(L)","W(cr)","W(L)","WC(cr)","WCL6(I)","WCL6(II)","WCL6(III)","WCL6(L)","WOCL4(cr)","WOCL4(L)","WO2(cr)","WO2(cr
)","WO2CL2(cr)","WO3(crIII)","WO3(crIII,II)","WO3(crI)","WO3(L)","Zn(cr)","Zn(L)","ZnSO4(a)","ZnSO4(a)","ZnSO4(b)","Zr(a)","Zr(b)","Zr(L)","ZrN(s)","ZrN(L)
","ZrO2(a)","ZrO2(b)","ZrO2(L)","Air","B2H6(L)","B5H9(L)","(CH2)x(s)","CH3NO2(L)","CH4(L)","CH3OH(L)","CH6N2(L)","C2H2(L),acetyle","CH3CN(L)","C2H4(
L)","C2H4O(L),ethyle","C2H6(L)","C2H5OH(L)","C2H8N2(L),UDMH","C2N2(L)","C3H6(L),propyle","C3H7NO3(L)","C3H8(L)","C4H8(L),1-buten","C4H10(L),n-
buta","C4H10(L),isobut","C5H12(L),n-pent","C6H6(L)","C6H5NH2(L)","C6H14(L),n-hexa","C7H8(L)","C7H16(L),n-hept","C8H18(L),n-
octa","C8H18(L),isooct","CLF3(L)","CLO3F","CLO3F(L)","CL2(L)","F2(L)","F2O(L)","HNO3(L)","H2(L)","H2O2(L)","IRFNA","JP-4","JP-5","Jet-A(L)","Jet-
A(g)","LiCLO4(s)","NF3(L)","NH3(L)","NH4CLO4(I)","NH4CLO4(II)","NH4NO3(IV)","NH4NO3(III)","NH4NO3(II)","NH4NO3(I)","NH4NO3(L)","N2(L)","N2H4(L)",
"N2O4(L)","O2(L)","O3(L)"};
public double R=8.31446261815324; // Universal gas constant  J/(kmolK)
public String name="nasa9.txt";
public String species_name="";
public String comment="";
public String optional_identification;
public String atomName[]=new String[5];
public double atomN[]=new double[5];
public String aFormula;
public int natom;
public int isgas;
public int n_intervals;
public String ref_date;
public double M;
public double dhf;
public double temperature_range[][];
public double cc[][];
public int ncc[];
public double aCp[][];
public double b1[];
public double b2[];
public double dH0[];
public double aDELHF;
public Atom atomList[];
 public nasa9_Data(String gname)
 {readData(gname);}
public static boolean isNull(Object obj) {
    return obj == null;
 }
public String readData(String gname)
{ boolean b=false;
BufferedReader fin;
int i=0;
String satom="";
String s11="";
String s12="";
String s13="";
String s14="";
String s15="";
String s1x="";
String s1y="";
                try{
                    fin=new BufferedReader(new FileReader(name));
  try{
                                try{
                                try{
                                try{
   while(fin != null)
```

```
{   // line 1
            s11=Text.readStringLine(fin);
            species_name=s11.substring(0,15);
            species_name= species_name.trim();
            comment=s11.substring(15);
            //line 2
             s12=Text.readStringLine(fin);
             s1x=s12.substring(0,2);
             s1x=s1x.trim();
             n_intervals=Integer.parseInt(s1x);
             temperature_range=new double[n_intervals][2];
            cc=new double[n_intervals][8];
            aCp =new double[n_intervals][8];
            b1=new double[n_intervals];
            b2=new double[n_intervals];
            dH0=new double[n_intervals];
            ncc=new int[n_intervals];
            optional_identification=s12.substring(3,9);
             s1x=s12.substring(10,18);
             s1x=s1x.trim();
             char cs1x=s1x.charAt(0);
             natom=0;
             if(Character.isLetter(cs1x)) {String s1z[]=s1x.split(" ",2);atomName[0]=s1z[0]; atomN[0]=Double.parseDouble(s1z[1]);natom++;}
             else  {atomName[0]=null; atomN[0]=0.0;}
             //System.out.println("chemical formula 1  atom name = "+atomName[0]+" atom number "+atomN[0]);
             s1x=s12.substring(18,26);
             s1x=s1x.trim();
             cs1x=s1x.charAt(0);
             if(Character.isLetter(cs1x)) {String s1z[]=s1x.split(" ",2);atomName[1]=s1z[0]; atomN[1]=Double.parseDouble(s1z[1]);natom++;}
             else  {atomName[1]=null; atomN[1]=0.0;}
             s1x=s12.substring(26,34);
             s1x=s1x.trim();
             cs1x=s1x.charAt(0);
             if(Character.isLetter(cs1x)) {String s1z[]=s1x.split(" ",2);atomName[2]=s1z[0]; atomN[2]=Double.parseDouble(s1z[1]);natom++;}
             else  {atomName[2]=null; atomN[2]=0.0;}
             s1x=s12.substring(34,42);
             s1x=s1x.trim();
             cs1x=s1x.charAt(0);
             if(Character.isLetter(cs1x)) {String s1z[]=s1x.split(" ",2);atomName[3]=s1z[0]; atomN[3]=Double.parseDouble(s1z[1]);natom++;}
             else  {atomName[3]=null; atomN[3]=0.0;}
             s1x=s12.substring(42,50);
             s1x=s1x.trim();
             cs1x=s1x.charAt(0);
             if(Character.isLetter(cs1x)) {String s1z[]=s1x.split(" ",2);atomName[4]=s1z[0]; atomN[4]=Double.parseDouble(s1z[1]);natom++;}
             else  {atomName[4]=null; atomN[4]=0.0;}
    aFormula="";
    int nA=0;
             for(int ii=0;ii<natom;ii++)
    {aFormula+=atomName[ii];
    nA=(int)atomN[ii];
    if(nA!=1) aFormula+=nA;
    }
    isgas=Integer.parseInt(s12.substring(51,52));
              M=Double.parseDouble(s12.substring(52,65));
             dhf=Double.parseDouble(s12.substring(65));
             aDELHF=dhf;
   // line 3
              if(n_intervals==0)
              {s13=Text.readStringLine(fin);}
             for(int ix=0;ix<n_intervals;ix++)
              {
              s13=Text.readStringLine(fin);
              temperature_range[ix][0]=Double.parseDouble(s13.substring(0,11));
              temperature_range[ix][1]=Double.parseDouble(s13.substring(11,22));
              ncc[ix]=Integer.parseInt(s13.substring(22,23));
              cc[ix][0]=Double.parseDouble(s13.substring(23,28));
              cc[ix][1]=Double.parseDouble(s13.substring(28,33));
              cc[ix][2]=Double.parseDouble(s13.substring(33,38));
              cc[ix][3]=Double.parseDouble(s13.substring(38,43));
              cc[ix][4]=Double.parseDouble(s13.substring(43,48));
              cc[ix][5]=Double.parseDouble(s13.substring(48,53));
```

```
                    cc[ix][6]=Double.parseDouble(s13.substring(53,58));
                    cc[ix][7]=Double.parseDouble(s13.substring(58,63));
                    dH0[ix]=Double.parseDouble(s13.substring(66));
                    // line 4
                    s14=Text.readStringLine(fin);
                    s1y=s14.substring(0,16);
                    s1y=s1y.replace('D','e');
                     s1y=s1y.trim();
                    aCp[ix][0]=Double.parseDouble(s1y);
                    s1y=s14.substring(16,32);
                    s1y=s1y.replace('D','e');
                     s1y=s1y.trim();
                    aCp[ix][1]=Double.parseDouble(s1y);
                    s1y=s14.substring(32,48);
                    s1y=s1y.replace('D','e');
                     s1y=s1y.trim();
                     aCp[ix][2]=Double.parseDouble(s1y);
                    //System.out.println("a3  = "+aCp[ix][2]);
                    s1y=s14.substring(48,64);
                    s1y=s1y.replace('D','e');
                    s1y=s1y.trim();
                     aCp[ix][3]=Double.parseDouble(s1y);
                    s1y=s14.substring(64);
                    s1y=s1y.replace('D','e');
                     s1y=s1y.trim();
                     aCp[ix][4]=Double.parseDouble(s1y);
                    // line 6
                     s15=Text.readStringLine(fin);
                     s1y=s15.substring(0,16);
                     s1y=s1y.replace('D','e');
                      s1y=s1y.trim();
                      aCp[ix][5]=Double.parseDouble(s1y);
                     s1y=s15.substring(16,32);
                     s1y=s1y.replace('D','e');
                      s1y=s1y.trim();
                      aCp[ix][6]=Double.parseDouble(s1y);
                    s1y=s15.substring(48,64);
                     s1y=s1y.replace('D','e');
                     s1y=s1y.trim();
                     b1[ix]=Double.parseDouble(s1y);
                    s1y=s15.substring(64);
                    s1y=s1y.replace('D','e');
                     s1y=s1y.trim();
                     b2[ix]=Double.parseDouble(s1y);
      }
      if(gname.equals(species_name))
      {  atomList=new Atom[natom];
        for(int ix=0;ix<natom;ix++)
        {atomList[ix]=new Atom(atomName[ix], atomN[ix]);}
                      return species_name;
                    }
      }
      } catch(ArrayIndexOutOfBoundsException e_eof) { }
      } catch(StringIndexOutOfBoundsException e_eof) { }
      } catch(EOFException e_eof) {System.out.println("end of file"); }
      } catch(NumberFormatException e_nfe) {System.out.println("non-number input"); }
      } catch(IOException e_io) {System.out.println("file name is not existed"); }
      return species_name;
}

public double Cp(double T)
{  double Cp1=0.0;
                for(int ix=0;ix<n_intervals;ix++)
   { if(T>= temperature_range[ix][0] && T<=temperature_range[ix][1])
     {   Cp1=aCp[ix][0]/(T*T)+aCp[ix][1]/(T)+aCp[ix][2]+aCp[ix][3]*T+aCp[ix][4]*T*T+aCp[ix][5]*T*T*T+aCp[ix][6]*T*T*T*T;
      Cp1*=R;

     return Cp1;
     }
   }
   System.out.println("given Temperature . "+T+" out of temperature range");
```

```
    return Cp1 ;
}

public double h1(double T)
{  double h1=0.0;
                for(int ix=0;ix<n_intervals;ix++)
   { if(T>= temperature_range[ix][0] && T<=temperature_range[ix][1])
     {h1=-
aCp[ix][0]/(T*T)+aCp[ix][1]/(T)*Math.log(T)+aCp[ix][2]+aCp[ix][3]*T/2.0+aCp[ix][4]*T*T/3.0+aCp[ix][5]*T*T*T/4.0+aCp[ix][6]*T*T*T*T/5.0+b1[ix]/T;
      h1=h1*R*T;
      h1+=dH0[ix];
     return h1;
     }
   }
    System.out.println("given Temperature . "+T+" out of temperature range");
    return h1 ;
}

public double u1(double T)
{ return h1(T)-R*T;}

//chemical enthalpy
public double ht(double T)
{  double h1=0.0;
                for(int ix=0;ix<n_intervals;ix++)
   { if(T>= temperature_range[ix][0] && T<=temperature_range[ix][1])
     {h1=-
aCp[ix][0]/(T*T)+aCp[ix][1]/(T)*Math.log(T)+aCp[ix][2]+aCp[ix][3]*T/2.0+aCp[ix][4]*T*T/3.0+aCp[ix][5]*T*T*T/4.0+aCp[ix][6]*T*T*T*T/5.0+b1[ix]/T;
      h1*=R*T;
     return h1;
     }
   }
    System.out.println("given Temperature . "+T+" out of temperature range");
    return h1 ;
}
public double st(double T,double P)
{return s(T,P)-s(298.15,P);}

public double h(double T)
{return h1(T)-dhf;}

public double s0(double T)
{  double s1=0.0;
                for(int ix=0;ix<n_intervals;ix++)
   { if(T>= temperature_range[ix][0] && T<=temperature_range[ix][1])
     {s1=-aCp[ix][0]/(2.0*T*T)-aCp[ix][1]/(T)+aCp[ix][2]*Math.log(T)+aCp[ix][3]*T+aCp[ix][4]*T*T/2.0+aCp[ix][5]*T*T*T/3.0+aCp[ix][6]*T*T*T*T/4.0+b2[ix];
      s1*=R;
     return s1;
     }
   }
    System.out.println("given Temperature . "+T+" out of temperature range");
    return s1 ;
}
public double s1(double T)
{ return s0(T);}

public double s(double T,double P)
{  double P0=101.325; //kPa
                return s0(T)-Math.log(P/P0);
}

public static void main(String arg[]) throws FileNotFoundException
{   nasa9_Data md=new nasa9_Data("CO2");
   PrintStream fout=new PrintStream(new FileOutputStream("nasa9_out.txt"));
   for(int i=0;i<md.name_list.length;i++)
   {fout.println(md.name_list[i]+" ");
    md=new nasa9_Data(md.name_list[i]);
    for(int j=0;j<md.n_intervals;j++)
    {   fout.print(j+" ");
                    for(int k=0;k<7;k++)
                    {fout.print(md.aCp[j][k]+" ");}
```

```
                    fout.println(md.b1[j]+" "+md.b2[j]+" "+md.aDELHF);
    }

    }
    fout.close();
    System.out.println("");
    /*
    System.out.println("\nspecies name : "+md.species_name);
    System.out.println("comment="+md.comment);
   System.out.println("n_intervals="+md.n_intervals);
   System.out.println("Optional identification code ="+md.optional_identification);
   System.out.println("chemical formula 1  atom name = "+md.atomName[0]+" atom number "+md.atomN[0]);
   System.out.println("chemical formula 2  atom name = "+md.atomName[1]+" atom number "+md.atomN[1]);
   System.out.println("chemical formula 3  atom name = "+md.atomName[2]+" atom number "+md.atomN[2]);
   System.out.println("chemical formula 4  atom name = "+md.atomName[3]+" atom number "+md.atomN[3]);
   System.out.println("chemical formula 5  atom name = "+md.atomName[4]+" atom number "+md.atomN[4]);
   System.out.println("natom="+md.natom);
   System.out.println("aFormula="+md.aFormula);
   for(int ix=0;ix<md.n_intervals;ix++)
   {   System.out.println("T1 = "+md.temperature_range[ix][0]+" T2 = "+md.temperature_range[ix][1]);
       System.out.println("number of coefficients for Cp  = "+md.ncc[ix]);
                    System.out.print("n1  = "+md.cc[ix][0]+" ");
                    System.out.print("n2  = "+md.cc[ix][1]+" ");
                    System.out.print("n3  = "+md.cc[ix][2]+" ");
                    System.out.print("n4  = "+md.cc[ix][3]+" ");
                    System.out.print("n5  = "+md.cc[ix][4]+" ");
                    System.out.print("n6  = "+md.cc[ix][5]+" ");
                    System.out.print("n7  = "+md.cc[ix][6]+" ");
                    System.out.println("n8  = "+md.cc[ix][7]+" ");
                    System.out.println("gas/condensed = "+md.isgas);
                    System.out.println("molecular weight = "+md.M);
                    System.out.println("heat of formation = "+md.dhf);
                     System.out.println("dH[0] = "+md.dH0[ix]);
                    System.out.print("Cp = "+md.aCp[ix][0]+" ");
                    System.out.print(md.aCp[ix][1]+" ");
                    System.out.print(md.aCp[ix][2]+" ");
                    System.out.print(md.aCp[ix][3]+" ");
                    System.out.print(md.aCp[ix][4]+" ");
                    System.out.print(md.aCp[ix][5]+" ");
                    System.out.print(md.aCp[ix][6]+" ");
                    System.out.println(md.aCp[ix][7]);
                    System.out.println("b1 = "+md.b1[ix]);
                     System.out.println("b2  = "+md.b2[ix]);
   }
        double T=1000;
                     double P=100;
                     System.out.println("Cp="+md.Cp(T));
                     System.out.println("h="+md.h(T));
                     System.out.println("hT="+md.ht(T));
                     System.out.println("sT="+md.st(T,P));
                     System.out.println("s0="+md.s0(T));
                     */
}
}
```

Gas_PG_nasa9

```
import java.io.*;
import javax.swing.*;
public class Gas_PG_nasa9
{public nasa9_Data gd;
 public Gas_Data gd1;
 boolean mole=true;
 public double M;
 public double R; // Universal gas constant  J/(kmolK)
 Atom atomList[];
 int natom;
 String Formula;
 String Name;
```

```
 double mu0=0;
 double P0=101.325;
 double T0=273.15;
   double v0,ro0,v0M;
 public double Tfp,Tb,Tc,Pc,Vc,roc,Zc,Omega,mu;
 public Gas_PG_nasa9(String gas_name)
 {  gas_name=gas_name.toUpperCase();
                gd=new nasa9_Data(gas_name);
                gd1=new Gas_Data();
    gd1=gd1.input(gas_name);
  M=gd.M;
  Tfp=gd1.Tfp;
  Tb=gd1.Tb;
  Tc=gd1.Tc;
  Vc=gd1.aVc;
  roc=11.0/Vc;
  Pc=gd1.Pc;
  Zc=gd1.aZc;
  R=8314.46261815324;
  natom=gd.natom;
  atomList=new Atom[natom];
  Formula=gd.aFormula;
  //Name=gd.aName;
  M=gd.M;
  for(int i=0;i<natom;i++)
 {atomList[i]=new Atom(gd.atomName[i],gd.atomN[i]);
 }
  }
  public double Cp(double T)
  {double Cp=gd.Cp(T);
    if(!mole) Cp/=M;
    return Cp;
  }

  public double Cv(double T)
  {double Cp=gd.Cp(T);
    double Cv=Cp-R*1e-3;
    if(!mole) Cv/=M;
    return Cv;
  }
 public double integCv(double T)
 { double iCv=gd.u1(T);
   if(!mole)  iCv/=M;
  return iCv;
 }
 public double integCp_T(double T)
 {  double iCp=gd.s1(T);
    if(!mole)  iCp/=M;
    return iCp;
 }
  public double integCp(double T)
 { double iCp=gd.h1(T);
   if(!mole)  iCp/=M;
  return iCp;
 }
 /*
 public double integCv_T(double T)
 {  double iCv=gd.s2(T);
    if(!mole)  iCv/=M;
    return iCv;
 }
 */
  public double h(double T)
  { double h=gd.h(T)-gd.h(273.15);
    if(!mole) h/=M;
    return h;
  }

  public double ht(double T)
  {double h=gd.h(T)-gd.h(298.15)+gd.aDELHF;
    if(!mole) h/=M;
```

```
    return h;
  }

  public double u(double T)
  {double h=gd.h(T)-gd.h(273.15);
  double T0=273.15;
    double u=h-R*1e-3*(T-T0);
    if(!mole) u/=M;
    return u;
  }
   public double st(double T,double P)
  {  double dS=0.0;//gd.aDELSF;
      if(!mole) dS/=M;
                double s0t=s(T,P)-s(298.15,P0)+dS;
    return s0t;
  }
   public double s0t(double T)
  { return st(T,P0);}

   public double s(double T,double P)
  { double s=gd.s0(T)-gd.s0(T0)-R*1e-3*Math.log(P/P0);
    if(!mole) s/=M;
    return s;
  }
 public double s(double T)
 {return s(T,P0)-s(T0,P0);}

 public double s0(double T)
 {return s(T);}

  public double P_Tv(double T,double v)
  {double P=R*T/v;
    if(!mole) P/=M;
    return P*1e-3;  //kPa
  }

  public double P_Tro(double T,double ro)
  {double P=R*T*ro;
    if(!mole) P/=M;
    return P*1e-3; //kPa
  }

  public double T_Pro(double P,double ro)
 {double T=P*1e3/(R*ro); //case of ideal gas
   if(!mole)  T/=M;
   return T;
  }
 public double T_h(double h)
 {if_x f1=x->h(x)-h;
 double T=secant(f1,T0);
 return T;
 }

 public double T_sP(double s,double P)
 {if_x f1=x->s(x,P)-s;
 double T=secant(f1,T0);
 return T;
 }

 public double P_Ts(double T,double s)
 {if_x f1=x->s(T,x)-s;
 double P=secant(f1,P0);
 return P;
 }

    public double T_Pv(double P,double v)
 {double T=P*1e3*v/R; //case of ideal gas
   if(!mole)  T/=M;
   return T;
  }
  public double v(double T,double P)
```

```
  {double v=R*T/(P*1.0e3);
     if(!mole) v/=M;
     return v;
  }

   public double ro(double T,double P)
  {double v=R*T/(P*1.0e3);
    if(!mole) v/=M;
    double ro=1.0/v;
     return ro;
  }


  //Gibbs free energy
  public double g(double T,double P)
{ return h(T)-T*s(T,P);
}

public double gt(double T,double P)
{ return ht(T)-T*st(T,P);}

public double gt0(double T)
{ return ht(T)-T*s0(T);}

  public double viscosity(double T)
  {return gd1.viscosity(T);}

  public double k(double T)
  {return gd1.k(T);}

public double Prandtl(double T)
{
// Prandtl number
double Cp=0;
if(mole) {Cp=Cp(T)/M;}
else {Cp=Cp(T);}
double Pr=0;
Pr=Cp*1.0e3*viscosity(T)/k(T);
return Pr;
}
double beta(double T,double ro)
{return 1.0/T;}

//Isothermal compresibility
public double dP_dv_Tro(double T,double ro)
{double v=1.0/ro;
 double v1=0;
 if(!mole) v1=v*M;
 else v1=v;
 double y=-R*T/(v1*v1);
 return y;
}
public double kappaS_Tro(double T,double ro)
{  double y1=dP_dv_Tro(T,ro);
   double v=1.0/ro;
    double v1=0;
    if(!mole) v1=v*M;
    else v1=v;
   double y=-1.0/y1/v1;
  return y;
}
//Isothermal compresibility
public double kappaS_TP(double T,double P)
{  double v=v(T,P);
   double ro=1.0/v;
   double y1=dP_dv_Tro(T,ro);
    double v1=0;
    if(!mole) v1=v*M;
    else v1=v;
   double y=-1.0/y1/v1;
  return y;
```

```
}
//speed of sound
public double a_T(double T)
{  double gamma=Cp(T)/Cv(T);
   double x=gamma*R/M*T;
   double a=Math.sqrt(x);
   return a;
}
public double w_T(double T)
{  double gamma=Cp(T)/Cv(T);
   double x=gamma*R/M*T;
   double a=Math.sqrt(x);
   return a;
}
public static double[] secant2(ifi_xj f,double x[])
{
// Roots of nonlinear system of equations secant method
//ti : weight function
//x vector of independent variables
//y vector of dependent variables
//dy derivative vector of dependent variables
double ti=1.0;
int i;
int nmax=20;
double tolerance=1.0e-4;
int n=x.length;
double b[];
b=new double[n];
for(i=0;i<n;i++)
{
b[i]=1.0;
}
i=0;
while( i++ < nmax && Matrix.abs(b) > tolerance )
{ b=Matrix.multiply(Matrix.divide(f.func(x),f.dfunc(x)),-ti);
  x=Matrix.add(x,b);
}
if(i >= nmax) System.out.println("Warning : Maximum number of iterations are exceeded \nResults may not be valid");
return x;
}
 public static double secant(if_x f,double x)
{ double eps=1.0e-6;
  double y=f.func(x);
  double dy=f.dfunc(x);
  int miter=100;
  int i=0;
  while(Math.abs(y)>eps && i<miter)
  {x=x-y/dy;
   y=f.func(x);
   dy=f.dfunc(x);
   i++;
  }
  if(i>=miter)
    System.out.println("i="+i+"result may not be correct");
  return x;
}
public double[] property_TP(double T,double P)
{double a[]=new double[17];
 double ro=ro(T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
```

```
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Pro(double P,double ro)
{double a[]=new double[17];
 double T=T_Pro(P,ro);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Tro(double T,double ro)
{double a[]=new double[17];
 double P=P_Tro(T,ro);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Ph(double P,double h)
{double a[]=new double[17];
 double T=T_h(h);
 double ro=ro( T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=0.0;//viscosity(T);
 a[12]=0.0;//k(T);
 a[13]=0.0;
 a[14]=0.0;//Prandtl(T);
 a[15]=ro;
```

```
 a[16]=w_T(T);
 return a;
}
public double[] property_Ps(double P,double s)
{double a[]=new double[17];
 double T=T_sP(s,P);
 double ro=ro( T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=0.0;//viscosity(T);
 a[12]=0.0;//k(T);
 a[13]=0.0;
 a[14]=0.0;//Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Ts(double T,double s)
{double a[]=new double[17];
 double P=P_Ts(T,s);
 double ro=ro( T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=0.0;//viscosity(T);
 a[12]=0.0;//k(T);
 a[13]=0.0;
 a[14]=0.0;//Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
        public double mu(double iT,double iP,double n,double nt){
                double mu=0;
                        double value=0;
                        double lnP=Math.log(iP/P0);
                        value=Math.abs(n)<1e-20? 0 :Math.log(n/nt);
                        mu=(gt(iT,P0)+8.3145*iT*value+8.3145*iT*lnP);
                return mu;
        }
        public void getmu0(double iT,double iP){
                mu0=gt0(iT);
        }
 public double[] property(String s,double v1,double v2)
{ if(s.equals("pt")) return property_TP(v2,v1);
 else if(s.equals("tp"))  {return property_TP(v1,v2);}
 else if(s.equals("vt"))  {double ro=1.0/v1;return property_Tro(v2,ro);}
 else if(s.equals("tv"))  {double ro=1.0/v2;return property_Tro(v1,ro);}
 else if(s.equals("rot")) {return property_Tro(v2,v1);}
 else if(s.equals("tro")) {return property_Tro(v1,v2);}
 else if(s.equals("pv"))  return property_Pro(v1,1.0/v2);
 else if(s.equals("pro")) return property_Pro(v1,v2);
 else if(s.equals("vp"))  return property_Pro(v2,1.0/v1);
 else if(s.equals("rop")) return property_Pro(v2,v1);
```

```
  else if(s.equals("ph"))  return property_Ph(v1,v2);
  else if(s.equals("hp"))  return property_Ph(v2,v1);
  else if(s.equals("ps"))  return property_Ps(v1,v2);
  else if(s.equals("sp"))  return property_Ps(v2,v1);
  //else if(s.equals("ts"))  return property_Ts(v1,v2);
  //else if(s.equals("st"))  return property_Ts(v2,v1);
  else return property_TP(v1,v2);
}
public double[] propertyC(String s,double v1,double v2)
{ double t=273.15;
  if(s.equals("pt")) return property_TP(v2,(v1+t));
  else if(s.equals("tp"))  {return property_TP((v1+t),v2);}
  else if(s.equals("vt"))  {double ro=1.0/v1;return property_Tro((v2+t),ro);}
  else if(s.equals("tv"))  {double ro=1.0/v2;return property_Tro((v1+t),ro);}
  else if(s.equals("rot")) {return property_Tro((v2+t),v1);}
  else if(s.equals("tro")) {return property_Tro((v1+t),v2);}
  else if(s.equals("pv"))  return property_Pro(v1,1.0/v2);
  else if(s.equals("pro")) return property_Pro(v1,v2);
  else if(s.equals("vp"))  return property_Pro(v2,1.0/v1);
  else if(s.equals("rop")) return property_Pro(v2,v1);
  else if(s.equals("ph"))  return property_Ph(v1,v2);
  else if(s.equals("hp"))  return property_Ph(v2,v1);
  else if(s.equals("ps"))  return property_Ps(v1,v2);
  else if(s.equals("sp"))  return property_Ps(v2,v1);
  else return property_TP((v1+t),v2);
}
public boolean input1()
{   Object[] o=new Object[]{"tp","vt","tv","rot","tro","pv","pro","vp","rop","ph","hp","ps","sp","quit"};
    String oname[]=new String[2];
    double v[]=new double[3];
    boolean b=true;
    ImageIcon picture=null;//new ImageIcon("fall.jpg");
    String option=(String)JOptionPane.showInputDialog(null,"Please select a known pair : ",
    "Input parameters of dry air ideal gas EOS",JOptionPane.QUESTION_MESSAGE,picture,o,"ATP");
     if(option.equals("tp")) {oname[0]="Temperature degree C";oname[1]="Pressure kPa";}
     else if(option.equals("vt")) {oname[1]="Temperature degree C";oname[0]="specific volume m^3/kg";}
     else if(option.equals("tv")) {oname[1]="Temperature degree C";oname[0]="specific volume m^3/kg";}
     else if(option.equals("rot")) {oname[1]="Temperature degree C";oname[0]="density kg/m^3";}
     else if(option.equals("tro")) {oname[0]="Temperature degree C";oname[1]="density kg/m^3";}
     else if(option.equals("pv")) {oname[0]="Pressure kPa";oname[1]="specific volume m^3/kg";}
     else if(option.equals("pro")) {oname[0]="Pressure kPa";oname[1]="density kg/m^3";}
     else if(option.equals("vp")) {oname[1]="Pressure kPa";oname[0]="specific volume m^3/kg";}
     else if(option.equals("rop")) {oname[1]="Pressure kPa";oname[0]="density kg/m^3";}
     else if(option.equals("ph")) {oname[0]="Pressure kPa";oname[1]="h enthalpy kJ/kg";}
     else if(option.equals("hp")) {oname[1]="Pressure kPa";oname[0]="h enthalpy kJ/kg";}
     else if(option.equals("ps")) {oname[0]="Pressure kPa";oname[1]="s entropy kJ/kgK";}
     else if(option.equals("sp")) {oname[1]="Pressure kPa";oname[0]="s entropy kJ/kgK";}
     else b=false;
    if(b)
    {
    for(int i=0;i<2;i++)
                {v[i] =Double.parseDouble(JOptionPane.showInputDialog(oname[i]));}
    print(option,v[0],v[1]);
    }
   return b;
}
public String toString()
{
//return the chemical symbol of the gas
String s="";
for(int i=0;i<natom;i++)
  s=s+atomList[i].toString();
return s;
}
public void printC(String s,double v1,double v2)
{String s1[][]=toStringC(s,v1,v2);
 String s3="Properties of dry air ideal gas EOS ";
 String s2[]={"array no","property name","dry air property","unit"};
 Text.print(s1,s2,s3);
}
public void print(String s,double v1,double v2)
```

```
{String s1[][]=toString(s,v1,v2);
 String s3="Properties of dry air ideal gas EOS based on NASA 9 database";
 String s2[]={"array no","property name","dry air property","unit"};
 Text.print(s1,s2,s3);
}
public String[][] toString(String s, double v1, double v2)
{  String s1[][]=new String[17][4];
   s1[0][1]="P, pressure       ";
   s1[1][1]="T, temperature     ";
   s1[2][1]="v, specific volume ";
   s1[3][1]="h, enthalpy       ";
   s1[4][1]="u, internal energy ";
   s1[5][1]="s, entropy        ";
   s1[6][1]="x, quality        ";
   s1[7][1]="Cp, specific heat at constant pressure ";
   s1[8][1]="Cv, specific heat at constant volume ";
   s1[9][1]=""+'\u03B1'+" isobaric thermal expansion coefficient ";
   s1[10][1]=""+'\u03BA'+" isothermal compressibility" ;
   s1[11][1]=""+'\u03B7'+" Dynamic viscosity" ;
   s1[12][1]="k Thermal conductivity" ;
   s1[13][1]=""+'\u03C3'+" Surface tension" ;
   s1[14][1]="Prandtl number" ;
   s1[15][1]=""+'\u03C1'+" density" ;
   s1[16][1]=" speed of sound" ;
   if(!mole)
   {
   s1[0][3]=" kPA         ";
   s1[1][3]=" deg K        ";
   s1[2][3]=" m"+'\u00B3'+"/kg       ";
   s1[3][3]=" KJ/kg        ";
   s1[4][3]=" KJ/kg        ";
   s1[5][3]=" KJ/kgK        ";
   s1[6][3]=" kg vap/kg mix ";
   s1[7][3]=" KJ/kgK";
   s1[8][3]=" KJ/kgK";
   s1[9][3]=" 1/K";
   s1[10][3]=" 1/Pa";
   s1[11][3]=" Pa.s";
   s1[12][3]=" W/mK";
   s1[13][3]=" N/m";
   s1[14][3]=" ";
   s1[15][3]=" kg/m"+'\u00B3';
   s1[16][3]=" m/s";
   }
   else{
   s1[0][3]=" kPA         ";
   s1[1][3]=" deg K        ";
   s1[2][3]=" m"+'\u00B3'+"/kmol       ";
   s1[3][3]=" KJ/kmol        ";
   s1[4][3]=" KJ/kmol        ";
   s1[5][3]=" KJ/kmolK        ";
   s1[6][3]=" kg vap/kg mix ";
   s1[7][3]=" KJ/kmolK";
   s1[8][3]=" KJkmolK";
   s1[9][3]=" 1/K";
   s1[10][3]=" 1/Pa";
   s1[11][3]=" Pa.s";
   s1[12][3]=" W/mK";
   s1[13][3]=" N/m";
   s1[14][3]=" ";
   s1[15][3]=" kmol/m"+'\u00B3';
   s1[16][3]=" m/s";
   }
  double pp[]=property(s,v1,v2);
for(int i=0;i<17;i++)
   {s1[i][2]=""+pp[i];}
    //s1[6][2]=phase(pp[6]);
for(int i=0;i<17;i++)
{s1[i][0]=""+i;}
return s1;
}
```

```
public String[][] toStringC(String s, double v1, double v2)
{  String s1[][]=new String[17][4];
   s1[0][1]="P, pressure       ";
   s1[1][1]="T, temperature     ";
   s1[2][1]="v, specific volume ";
   s1[3][1]="h, enthalpy       ";
   s1[4][1]="u, internal energy ";
   s1[5][1]="s, entropy        ";
   s1[6][1]="x, quality        ";
   s1[7][1]="Cp, specific heat at constant pressure ";
   s1[8][1]="Cv, specific heat at constant volume ";
   s1[9][1]=""+'\u03B1'+" isobaric thermal expansion coefficient ";
   s1[10][1]=""+'\u03BA'+" isothermal compressibility" ;
   s1[11][1]=""+'\u03B7'+" Dynamic viscosity" ;
   s1[12][1]="k Thermal conductivity" ;
   s1[13][1]=""+'\u03C3'+" Surface tension" ;
   s1[14][1]="Prandtl number" ;
   s1[15][1]=""+'\u03C1'+" density" ;
   s1[16][1]=" speed of sound" ;
   if(!mole)
   {
   s1[0][3]=" kPA         ";
   s1[1][3]=" deg K        ";
   s1[2][3]=" m"+'\u00B3'+"/kg       ";
   s1[3][3]=" KJ/kg        ";
   s1[4][3]=" KJ/kg        ";
   s1[5][3]=" KJ/kgK        ";
   s1[6][3]=" kg vap/kg mix ";
   s1[7][3]=" KJ/kgK";
   s1[8][3]=" KJ/kgK";
   s1[9][3]=" 1/K";
   s1[10][3]=" 1/Pa";
   s1[11][3]=" Pa.s";
   s1[12][3]=" W/mK";
   s1[13][3]=" N/m";
   s1[14][3]=" ";
   s1[15][3]=" kg/m"+'\u00B3';
   s1[16][3]=" m/s";
   }
   else{
   s1[0][3]=" kPA         ";
   s1[1][3]=" deg K        ";
   s1[2][3]=" m"+'\u00B3'+"/kmol       ";
   s1[3][3]=" KJ/kmol        ";
   s1[4][3]=" KJ/kmol        ";
   s1[5][3]=" KJ/kmolK        ";
   s1[6][3]=" kg vap/kg mix ";
   s1[7][3]=" KJ/kmolK";
   s1[8][3]=" KJkmolK";
   s1[9][3]=" 1/K";
   s1[10][3]=" 1/Pa";
   s1[11][3]=" Pa.s";
   s1[12][3]=" W/mK";
   s1[13][3]=" N/m";
   s1[14][3]=" ";
   s1[15][3]=" kmol/m"+'\u00B3';
   s1[16][3]=" m/s";
   }
  double pp[]=propertyC(s,v1,v2);
for(int i=0;i<17;i++)
   {s1[i][2]=""+pp[i];}
    //s1[6][2]=phase(pp[6]);
for(int i=0;i<17;i++)
{s1[i][0]=""+i;}
return s1;
}
public static void main(String arg[])
{Gas_PG_nasa9 pr=new Gas_PG_nasa9("N2");
 Gas_PG pr1=new Gas_PG("N2");
  double T=273.15; //degree K
  double P=1000; //kPa
```

```
  double T1[]=new double[500];
  double h1[]=new double[500];
  for(int i=0;i<500;i++)
    {
    T1[i]=273.15+2.0*i;
    h1[i]=Math.abs(pr.s(T1[i],P)-pr1.s(T1[i],P));
    }
  Plot p=new Plot(T1,h1);
  p.plot();

  //pr.print("tp",T,P);
  //pr1.print("tp",T,P);
  //double a[]=pr.property("tp",T,P);
  //for( double x :a) System.out.println(x);
 }


 }
```

Gas_Data

```
import java.io.*;
import java.util.*;
public class Gas_Data
{public  int ierror;
   public int i;
   public boolean mole=true;
   String atomName[];  //Name of the Atoms defined at Atom.java
   boolean includeCH;
   String names[];

   String formulas[];
   double atomN[];
   int anatom;
   String tempName="";
   String tempFormula="";
   String aFormula,formula;
   String aName,name;
   int aNo;
   public double T0=273.15; //degree K
   public double P0=101.325; //kPA
   public int aCpEq;
   double aMolWt,aTfp,aTb,aTc,aPc,aVc,aZc,aOmega,aDipm;
   public double M,Tfp,Tb,Tc,Pc,Vc,Zc,Omega,mu,w;
   // M kg/kmol  molar weight
   // Tfp freezing point (at 101.325 kPa) degree K
   // Tb boiling point  (at 101.325 kPa) degree K
   // Tc  critical temperature degree K
   // Pc critical presssure bar
   // Vc critical volume cm^3/mol
   // Zc critical compressibility factor
   // aOmega Pitzers acentricity factor
   // aDipm  Dipole moment Debys
   // mu       Dipole moment Debys
   double aCPC[]=new double[4];
   double aDELHF,aDELGF,aDELSF;
   int aVPEq;
   double aVPC[]=new double[4];
   double aTmin,aTmax,aLDEN,aTDEN ;
   Vector<Gas_Data> gi;//=new Vector<Gas_Data>();
   //partial continious Cp data
   double xa[],xb[],xc[],xd[],tl[],th[];
   int n_equation;
   //Viscosity and thermal conductivity
   double xvis[];
   double xk[];
   public double R=8314.46261815324; // Universal gas constant  J/(kmolK)
                              public boolean isCH()
                              {int ii=0;
```

```
                                boolean isCH=false;
                                for(int i=0;i<atomName.length;i++)
        {if(atomName[i].equals("H")) ii++;
          else if(atomName[i].equals("C")) ii++;
        }
        if(ii>=2) isCH=true;
        return isCH;
        }
   public void input1(int aNo,String aFormula,String aName,String atomName[],double atomN[])
  {this.aNo=aNo;this. aFormula= aFormula;formula=aFormula;this.aName= aName;name=aName;this.atomName=atomName;this.atomN=atomN;double
xvis1[]={};xvis=xvis1;double xk1[]={};xk=xk1;}

  public void input2(double aMolWt,double aTfp,double aTb,double aTc,double aPc,double aVc,double aZc,double aOmega,double aDipm )
  {this.aMolWt=aMolWt;M=aMolWt;this.aTfp=aTfp;Tfp=aTfp;this.aTb=aTb;Tb=aTb;this.aTc=aTc;Tc=aTc;this.aPc=aPc;Pc=aPc*1e2;this.aVc=aVc*1e-
3;Vc=aVc;this.aZc=aZc;Zc=aZc;this.aOmega=aOmega;w=aOmega;this.aDipm=aDipm;mu=aDipm; }

  public void input3(int aCPeqi,double aCPC[])
  {aCpEq=aCPeqi;this.aCPC=aCPC;}

    public void input4(int aVPEq,double aVPC[])
  {this.aVPEq=aVPEq;this.aVPC=aVPC;}

public void input5(double aDELHF,double aDELGF)
{this.aDELHF=aDELHF;this.aDELGF=aDELGF;aDELSF=(aDELHF-aDELGF)/298.15;}

public void inputCp(double ixa[][])
{n_equation=ixa.length;
aCpEq=2;
xa=new double[n_equation];
xb=new double[n_equation];
xc=new double[n_equation];
xd=new double[n_equation];
tl=new double[n_equation];
th=new double[n_equation];
for(int i=0;i<n_equation;i++)
{
 xa[i]=ixa[i][0];
 xb[i]=ixa[i][1];
 xc[i]=ixa[i][2];
 xd[i]=ixa[i][3];
 tl[i]=ixa[i][4];
 th[i]=ixa[i][5];
}
}

public void input_visc(double amu[])
{  xvis=amu;}

public void input_k(double ak[])
{xk=ak;}

  public void data1()
  {Gas_Data gd=new Gas_Data();
String atomName1[]={"N","H"};atomName=atomName1;double atomN1[]={1.0,3.0};atomN=atomN1;
gd.input1(1,"NH3","ammonia",atomName,atomN);
gd.input2(17.031,195.4,239.8,405.5,113.5,72.5,0.244,0.25,1.5);
double aCPC1[]={27.31,0.02383,1.707E-5,-1.185E-8};aCPC=aCPC1;gd.input3(1,aCPC);
double aVPC1[]={45.327,4104.67,-5.146,615.0};aVPC=aVPC1;gd.input4(2,aVPC);
gd.input5(-45720.0,-16160.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName2[]={"Ar"};atomName=atomName2;double atomN2[]={1.0};atomN=atomN2;
gd.input1(2,"Ar","argon",atomName,atomN);
gd.input2(39.948,83.8,87.3,150.8,48.7,74.9,0.291,0.0,0.0);
double aCPC2[]={20.8,0.0,0.0,0.0};aCPC=aCPC2;gd.input3(1,aCPC);
double aVPC2[]={-5.90501,1.12627,-0.76787,-1.62721};aVPC=aVPC2;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
```

```
String atomName3[]={"C","H","Cl"};atomName=atomName3;double atomN3[]={6.0,5.0,1.0};atomN=atomN3;
gd.input1(3,"C6H5Cl","chlorobenzene",atomName,atomN);
gd.input2(112.559,227.6,404.9,632.4,45.2,308.0,0.265,0.249,1.6);
double aCPC3[]={-33.89,0.5631,-4.522E-4,1.426E-7};aCPC=aCPC3;gd.input3(1,aCPC);
double aVPC3[]={-7.587,2.26551,-4.09418,0.17038};aVPC=aVPC3;gd.input4(1,aVPC);
gd.input5(51870.0,99230.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName4[]={"N","O"};atomName=atomName4;double atomN4[]={1.0,1.0};atomN=atomN4;
gd.input1(4,"NO","nitricoxide",atomName,atomN);
gd.input2(30.006,109.5,121.4,180.0,64.8,57.7,0.25,0.588,0.2);
double aCPC4[]={29.35,-9.378E-4,9.747E-6,-4.187E-9};aCPC=aCPC4;gd.input3(1,aCPC);
double aVPC4[]={24.097,1408.77,-2.579,336.0};aVPC=aVPC4;gd.input4(2,aVPC);
gd.input5(90291.0,86600.0);
double agNO[][]={{33.06470671449779,-21.269110442793636,0.1026056059465571,33.814850059272956,100.0,300.0},
{28.507125706890548,-1.910010933766341,0.8796716480496226,10.329468963512923,300.0,500.0},
{20.88783380194883,19.818962109277045,3.6622151511843333,-7.105271267053868,500.0,900.0},
{29.078203580684043,7.623159755846156,-7.50631411577063,-1.9634586588537664,900.0,1300.0},
{33.690127460043215,2.767724467164074,-19.916980809037497,-0.5228637571051207,1300.0,1700.0},
{35.914942110580476,0.972421145071174,-30.047821068952494,-0.11535487198801654,1700.0,2100.0},
{35.630599922571434,1.1186351436273005,-26.804248923987185,-0.13716665788909274,2100.0,2500.0},
{36.24984852360516,0.7222442919725142,-30.722509087178683,-0.06765783393781291,2500.0,2900.0},
{30.95445483518726,2.948196840764959,57.08222809827734,-0.32971790219504904,2900.0,3300.0},
{45.69448274798853,-2.9554888576114995,-217.3452749936191,0.33713985024094534,3300.0,3700.0},
{35.677990670013585,0.7550031927700818,2.355376917162876E-4,-0.05000030705973665,3700.0,4100.0},
{25.94191460810105,3.7354659632323846,307.41191382316293,-0.3065486024002062,4100.0,4500.0},
{36.06493973218778,0.5523564588393092,7.234491873390216,-0.02589119621658216,4500.0,4900.0},
{53.158071826453174,-3.9456742877261006,-721.4982551467294,0.3065695855710619,4900.0,5300.0},
{77.55947637936835,-9.51930284480678,-2077.6235714544623,0.6613780891303459,5300.0,5700.0},
{36.96629516334837,0.2503886625369599,0.09713346015991346,-2.4915430046628612E-5,5700.0,6000.0}};
gd.inputCp(agNO);
double avisiNO[]={399.21,5.37,-1.24e-3};
double akiNO[]={1.176,8.2369e-2,-1.2527e-5};
gd.input_visc( avisiNO);
gd.input_k(akiNO);
gi.addElement(gd);

gd=new Gas_Data();
String atomName5[]={"N","O"};atomName=atomName5;double atomN5[]={1.0,2.0};atomN=atomN5;
gd.input1(5,"NO2","nitrogendioxide",atomName,atomN);
gd.input2(46.006,261.9,294.3,431.0,101.0,167.8,0.473,0.834,0.4);
double aCPC5[]={24.23,0.04836,-2.081E-5,2.93E-10};aCPC=aCPC5;gd.input3(1,aCPC);
double aVPC5[]={55.242,6073.34,-6.094,780.0};aVPC=aVPC5;gd.input4(2,aVPC);
double avisiNO2[]={-3723.75,23.3,-2.15e-2};
double akiNO2[]={-1.289,1.039e-3,-2.1445e-5};
gd.input_visc( avisiNO2);
gd.input_k(akiNO2);
gd.input5(33095.0,51258.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName6[]={"N"};atomName=atomName6;double atomN6[]={2.0};atomN=atomN6;
gd.input1(6,"N2","nitrogene",atomName,atomN);
gd.input2(28.013,63.3,77.4,126.2,33.9,89.8,0.29,0.039,0.0);
double aCPC6[]={31.15,-0.01357,2.68E-5,-1.168E-8};aCPC=aCPC6;gd.input3(1,aCPC);
double aVPC6[]={-6.09676,1.1367,-1.04072,-1.93306};aVPC=aVPC6;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
double agN2[][]={{29.246342790518764,-1.1138715372079058,-0.005526874556677223,2.4313004958059015,100.0,300.0},
{30.692531648559026,-8.3543286890773,-0.17007726325583347,12.531067177424816,300.0,500.0},
{21.72477341276599,14.401836022352443,4.022586836653579,-3.8179584511038915,500.0,900.0},
{24.687198794462855,10.886167793274725,-1.5334783410749462,-2.7228108984500454,900.0,1300.0},
{30.30371151980031,5.001930403092595,-16.797140364584205,-0.9853948226394288,1300.0,1700.0},
{33.425942073410745,2.430588058935691,-30.615395772466222,-0.3877320985322228,1700.0,2100.0},
{36.52020032642022,0.4422700075660129,-53.60850204312567,-0.02433327016254659,2100.0,2500.0},
{39.444406340569735,-0.9799150294000134,-89.82386561251856,0.1693757332087812,2500.0,2900.0},
{36.80383031433077,0.3524058467404462,-59.805464604302706,-0.01851034056124957,2900.0,3300.0},
{34.072307648040116,1.368380861625423,-2.2173664302689033,-0.12411170689849348,3300.0,3700.0},
{34.79111637090394,0.9914877870163281,-3.4218899620517296,-0.07411241152418199,3700.0,4100.0},
{55.00538668203772,-5.360479546559665,-609.7585773985858,0.48720607356356516,4100.0,4500.0},
{36.16292841512774,0.35002032141849765,0.0026279208446306325,-1.6216471248137908E-6,4500.0,4900.0},
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{-14.524351986549025,13.732811196901995,2154.467732898691,-0.9938210959047827,4900.0,5300.0},
{59.65187308131886,-5.663287095930621,-1052.384863286962,0.4315783790669697905,5300.0,5700.0},
{-11.643388988748901,10.937517255473647,2851.4184751959165,-0.6562867059994574,5700.0,6000.0}};
gd.inputCp(agN2);
gi.addElement(gd);
double avisiN2[]={-7.01963701225759,0.858327699273598,-0.00112340740644438,1.4031330184525E-6,-1.2471558843147E-9,7.37784281928769E-13,-
2.73840279340566E-16,5.73795735055663E-20,-5.15666835382267E-24};
double akiN2[]={2.74464219691575,0.032560938823238,5.61143449732873E-4,-2.65097510427981E-6,6.32147739080813E-9,-8.64030177972148E-
12,6.79049143882341E-15,-2.84261270585969E-18,4.90168626035256E-22};
gd.input_visc( avisiN2);
gd.input_k(akiN2);

gd=new Gas_Data();
String atomName7[]={"N","O"};atomName=atomName7;double atomN7[]={2.0,1.0};atomN=atomN7;
gd.input1(7,"N2O","nitrousoxide",atomName,atomN);
gd.input2(44.013,182.3,184.7,309.6,72.4,97.4,0.274,0.165,0.2);
double aCPC7[]={21.62,0.07281,-5.778E-5,1.83E-8};aCPC=aCPC7;gd.input3(1,aCPC);
double aVPC7[]={39.824,2867.98,-4.655,557.0};aVPC=aVPC7;gd.input4(2,aVPC);
gd.input5(82048.0,104179.0);
double agN2O[][]={{15.837110028852324,101.32295061832228,0.42693515072762644,-88.97569216943455,100.0,300.0},
{26.93733205723148,51.414330656572076,-1.2470246298122536,-25.279690315250523,300.0,500.0},
{33.71154666891525,33.893107466367915,-4.365757875026845,-12.344506937030982,500.0,900.0},
{47.268091632128886,13.342109526471981,-22.256741109167688,-3.518970176699781,900.0,1300.0},
{55.526163663506814,4.63115258384996,-44.441326099452056,-0.9277940383139889,1300.0,1700.0},
{58.95788389269775,1.875898150831236,-60.28483183774019,-0.30483553016304854,1700.0,2100.0},
{61.39080223760698,0.3635055797829293,-79.18435123843624,-0.03914029895191969,2100.0,2500.0},
{61.968264520604386,0.10843834710077724,-87.48017278927178,-0.008275209931395957,2500.0,2900.0},
{67.75447468582628,-2.387775454987395,-179.41613527289036,0.2944681304547475,2900.0,3300.0},
{68.54576575596501,-2.4120985971773767,-219.56214104742463,0.2630271359608437,3300.0,3700.0},
{58.40082721848299,1.32853151936952,3.4233137111722534,-0.12588944546646244,3700.0,4100.0},
{68.9804219902619,-2.0650510420059036,-302.350369906387,0.1806607387213082,4100.0,4500.0},
{59.87290102371135,0.6650280974215728,0.0036334325796401417,-0.050002242184440465,4500.0,4900.0},
{43.571862736617554,4.880691410250632,721.5010832217938,-0.3565708451220564,4900.0,5300.0},
{39.346287573804545,5.5882481292750725,1052.3767809879173,-0.3815757218842709,5300.0,5700.0},
{110.6384327586923,-11.011843301430144,-2851.250044974605,0.7062435015838048,5700.0,6000.0}};
gd.inputCp(agN2O);
double avisiN2O[]={56.8,5.56,-1.52e-3};
double akiN2O[]={-6.03,7.9837e-2,-2.2582e-6};
gd.input_visc( avisiN2O);
gd.input_k(akiN2O);
gi.addElement(gd);

gd=new Gas_Data();
String atomName8[]={"O"};atomName=atomName8;double atomN8[]={2.0};atomN=atomN8;
gd.input1(8,"O2","oxygen",atomName,atomN);
gd.input2(31.999,54.4,90.2,154.6,50.4,73.4,0.288,0.025,0.0);
double aCPC8[]={28.11,-3.68E-6,1.746E-5,-1.065E-8};aCPC=aCPC8;gd.input3(1,aCPC);
double aVPC8[]={-6.28275,1.73619,-1.81349,-0.0253645};aVPC=aVPC8;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
double agO2[][]= {{30.365631005636665,-10.730151790122664,-0.0440763774381525,25.414790616774532,100.0,300.0},
{24.214805126942743,13.5583635444284,1.104145821180898,-1.3768867922683914,300.0,500.0},
{23.15156263499761,19.01905888035364,0.7046921141397134,-7.409045410904957,500.0,900.0},
{33.31982017023971,3.3262298777786548,-12.248322248128321,-0.5510253070465407,900.0,1300.0},
{36.76490495683016,-0.35035326916686405,-21.332108152717378,0.5566754995950703,1300.0,1700.0},
{33.482323745241466,2.2313295304930025,-5.323289935249809,-0.01776870438165389 2,1700.0,2100.0},
{30.901701501243014,3.861548772565201,13.811584080947343,-0.30729671875373155,2100.0,2500.0},
{26.80373407124348,5.969940895906629,59.88251728669684,-0.6129168140279246,2500.0,2900.0},
{27.47517961942772,5.50258987341556,59.805306600174795,-0.5314891414483293,2900.0,3300.0},
{31.76457717371467,3.611776265213672,-4.433958736577499,-0.29822497247502067,3300.0,3700.0},
{47.99373650563209,-2.204198487085609,-380.7089684463779,0.2889537682564038,3700.0,4100.0},
{45.121591803543865,-1.2795843599755874,-297.28370450904623,0.2047683599054678,4100.0,4500.0},
{65.22333806424805,-7.307815184951247,-959.2094794361566,0.7131206324306115,4500.0,4900.0},
{58.9608489776645,-5.5913686122672,-711.4556847248869,0.5806750109301544,4900.0,5300.0},
{88.71531245625047,-13.091711547820871,-2104.798214933699,1.113166124757938,5300.0,5700.0},
{49.36541955214663,-3.8296396968893007,0.0900472359973144,0.4999769026768179,5700.0,6000.0}};
gd.inputCp(agO2);
double avisiO2[]={-15.2819046089901,1.05385147522418,-0.00162349107208735,2.77516859994582E-6,-3.58520001415248E-9,3.10021571553767E-12,-
1.65985810687716E-15,4.93745323575399E-19,-6.2166840764683E-23};
double akiO2[]={-2.03305576203544,0.123232902604801,-1.32156973422579E-4,1.04767440853954E-7,1.6553201252612E-10,-5.17627201737314E-
13,5.42871301595178E-16,-2.63481619947786E-19,4.95504765460086E-23};
gd.input_visc(avisiO2);
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gd.input_k(akiO2);
gi.addElement(gd);

gd=new Gas_Data();
String atomName9[]={"O"};atomName=atomName9;double atomN9[]={3.0};atomN=atomN9;
gd.input1(9,"O3","ozone",atomName,atomN);
gd.input2(47.998,80.5,181.2,261.1,55.7,88.9,0.228,0.691,0.6);
double aCPC9[]={20.54,0.08009,-6.243E-5,1.697E-8};aCPC=aCPC9;gd.input3(1,aCPC);
double aVPC9[]={9.1225,1272.18,-22.16,0.0};aVPC=aVPC9;gd.input4(3,aVPC);
double agO3[][]= {{23.377856379500642,55.31437590111072,0.4510300720173685,-12.75911563180313,100.0,400.0},
{34.083282926753576,40.491065946253784,-5.471070659213091,-19.485064933715734,400.0,800.0},
{52.68616309358605,6.375796475006959,-22.192348413318385,-1.8211762301757155,800.0,1200.0},
{54.63983917868774,3.607257612920614,-24.381925499137008,-0.764955205967294,1200.0,1600.0},
{53.22426721928933,4.1590390778989015,-11.73436633012648,-0.7497360747408874,1600.0,2000.0},
{69.33100596804485,-6.298384162537761,-126.96125607669573,1.1724504552460666,2000.0,2400.0},
{55.128252493781524,2.000387439956222,-1.3422762730505085,-0.19823391630775877,2400.0,2800.0},
{62.14252952598284,-1.2437167436043897,-97.92170593314715,0.22280920869706414,2800.0,3200.0},
{11.863295005965673,18.784355096217695,840.810127477594,-2.0211125819255624,3200.0,3600.0},
{84.16495879854709,-8.597067830349468,-662.6309573324316,0.9011133042062128,3600.0,4000.0},
{102.70186041868553,-13.540355305325033,-1357.2038149524224,1.249693379947614,4000.0,4400.0},
{116.19787602214417,-16.26969132997005,-2087.1811224195867,1.3676370781353677,4400.0,4800.0},
{58.014559057220886,0.5374910500472099,-18.530234382382258,0.0017779745965501332,4800.0,5200.0},
{78.00189324464328,-4.444697975587102,-972.7864631021326,0.3512263139883577 4,5200.0,5600.0},
{56.05859075277329,0.8408900529731155,167.96506654820098,-0.008911073591938871,5600.0,6000.0}};
gd.inputCp(agO3);
double avisiO3[]={4.025721319116347,
0.4424434618132939,
7.179357425115897E-4,
-2.6605240568321E-6,
4.290947681391062E-9,
-4.146279561295185E-12,
2.5594084888285185E-15,
-1.0165270943469358E-18,
2.5139638730069E-22,
-3.522555430611318E-26,
2.1358822008912843E-30};
double akiO3[]={1.2851245465921919,
0.001156174168932887,
2.6706510780409343E-4,
-5.768405271177716E-7,
7.512017972770469E-10,
-6.595220530176374E-13,
3.900297961251671E-16,
-1.5129550384387958E-19,
3.6884821788274626E-23,
-5.1200385287843544E-27,
3.0842025201567854E-31};
gd.input_visc( avisiO3);
gd.input_k(akiO3);
gd.input5(142674.0,163184.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName10[]={"H"};atomName=atomName10;double atomN10[]={2.0};atomN=atomN10;
gd.input1(10,"H2","hydrogen",atomName,atomN);
gd.input2(2.016,14.0,20.3,33.0,12.9,64.3,0.303,-0.216,0.0);
double aCPC10[]={27.14,0.009274,-1.381E-5,7.645E-9};aCPC=aCPC10;gd.input3(1,aCPC);
double aVPC10[]={-5.57929,2.60012,-0.85506,1.70503};aVPC=aVPC10;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
double agH2[][]={{11.508997060028037,98.68272534099832,0.8241443728964292,-146.47147075487408,298.0,300.0},
{33.54524867881161,-12.210857124598489,-1.7456396844212596,10.074433281107176,300.0,500.0},
{31.07421577186371,-5.175597133082082,-0.8173138337326622,4.402304012148266,500.0,900.0},
{23.245582828841485,6.364182202934712,10.028643525215026,-0.40789312258308535,900.0,1300.0},
{19.853650144919794,10.069197699685896,18.50185307134015,-1.5475969619464518,1300.0,1700.0},
{22.835676520106627,7.6718371700950065,4.755713445416609,-1.0046084800067425,1700.0,2100.0},
{30.352200255524124,2.974004438611988,-52.78955672686392,-0.17609364991614967,2100.0,2500.0},
{25.659289152360312,5.3827829284053985,0.7811937079565058,-0.5258834350203144,2500.0,2900.0},
{34.71737612162783,1.0392087292970071,-116.88770293127145,0.0612075951047709,2900.0,3300.0},
{28.90471608012268,3.2516100869344826,2.216884622217297,-0.17588732290115694,3300.0,3700.0},
{36.98294018253396,0.4036399461542716,-192.06577611506046,0.1074211307913159,3700.0,4100.0},
{28.996598415560683,3.120853048671733,10.125384478047936,-0.1517777515076703,4100.0,4500.0},
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{15.010891525111804,7.314051049897713,472.37023762718,-0.5056691131905932,4500.0,4900.0},
{25.828874378877703,4.500032863027445,0.005431634761202251,-0.30000241688308116,4900.0,5300.0},
{23.072963880407887,5.550008760318859,0.0018172978589971332,-0.40000059734707977,5300.0,5700.0},
{70.70655920176688,-5.0080120092273255,-2851.542125388009,0.2563184222347695,5700.0,6000.0}};
gd.inputCp(agH2);
double avisiH2[]={2.20821838055369,0.506980026395776,-0.00138019011996754,3.33648388844839E-6,-4.91516640898999E-9,4.34474801305987E-
12,-2.25000324346063E-15,6.28027257836331E-19,-7.28348681229068E-23};
double akiH2[]={-20.9811386435507,1.0769371545451,-0.00238706110811684,5.26186077214256E-6,-7.66004998358933E-9,6.96248035011081E-12,-
3.72842468870476E-15,1.0718592543995E-18,-1.27416628164376E-22};
gd.input_visc( avisiH2);
gd.input_k(akiH2);

gi.addElement(gd);

gd=new Gas_Data();
String atomName11[]={"H","O"};atomName=atomName11;double atomN11[]={2.0,1.0};atomN=atomN11;
gd.input1(11,"H2O","water",atomName,atomN);
gd.input2(18.015,273.2,373.2,647.3,221.2,57.1,0.235,0.334,1.8);
double aCPC11[]={32.24,0.001924,1.055E-5,-3.596E-9};aCPC=aCPC11;gd.input3(1,aCPC);
double aVPC11[]={-7.76451,1.45838,-2.7758,-1.23303};aVPC=aVPC11;gd.input4(1,aVPC);
gd.input5(-241826.0,-228582.0);
double agH2O[][]= {{33.25219299471233,-1.0869505509180986,0.008208296694573765,7.341909343373295,100.0,300.0},
{29.127982455916964,10.642631579636186,1.0294736842726413,1.4596491222299655,300.0,600.0},
{28.614236360226595,11.633818187977187,1.4779112757087844,0.8887272696365881,600.0,900.0},
{20.67445214275589,23.667018373867247,11.817719563378859,-4.2552424729714575,900.0,1200.0},
{21.062298962123926,23.636712701413288,9.150276226727847,-4.370687536734363,1200.0,1500.0},
{28.4294045026366,17.271641842703737,-20.103000227106183,-2.823733595529846,1500.0,1800.0},
{68.24107462328517,-10.868431006571445,-255.91068842346112,2.768388650083263,1800.0,2100.0},
{40.774906547136936,8.54664742403356,-95.39757782957692,-1.0740716000341166,2100.0,2400.0},
{49.09712023197981,4.001668755141955,-178.6652037738798,-0.3741838176465953,2400.0,2700.0},
{47.350183036793105,4.838335259198056,-155.96769448925178,-0.4871349368102726,2700.0,3000.0},
{22.862611949396502,15.071698808412426,257.4720951420907,-1.687834381261323,3000.0,3300.0},
{71.73415069240694,-4.939901334465408,-609.020787455237,0.6191920201717109,3300.0,3600.0},
{16.896014001174215,15.071639543545274,616.331910421964,-1.4377749857397182,3600.0,3900.0},
{44.832973602779845,4.900008694425029,7.200713395655248E-4,-0.40000080507270447,3900.0,4200.0},
{66.77089094701616,-2.0483286778929077,-647.6993536717218,0.21886930519675468,4200.0,4500.0},
{22.058555285120306,11.023111331243765,904.2458034027555,-0.8563440815820761,4500.0,4800.0},
{58.540090945293436,-0.8300245055902843,-0.003708282834432604,0.20000185661338735,4800.0,5100.0},
{88.95693496151813,-7.7427849226775365,-1659.465414568823,0.6313100171911288,5100.0,5400.0},
{53.492469225072156,1.1798872466161838,-0.024061429165222848,7.618581743311251E-6,5400.0,5700.0},
{4.320975506094123,12.292662124088588,2851.4546890275697,-0.7062959921419553,5700.0,6000.0}};
gd.inputCp(agH2O);
double avisiH2O[]={0.620039710415251,0.236733467320225,3.34578658760477E-4,-2.81676758094982E-7,8.57370742701562E-11};
double akiH2O[]={9.79578978098437,-0.00571790459190282,1.36242662282321E-4,-4.13488699966119E-8,-1.06237803964109E-12};
gd.input_visc( avisiH2O);
gd.input_k(akiH2O);
gi.addElement(gd);

gd=new Gas_Data();
String atomName12[]={"C","H"};atomName=atomName12;double atomN12[]={1.0,4.0};atomN=atomN12;
gd.input1(12,"CH4","methane",atomName,atomN);
gd.input2(16.043,90.7,111.6,190.4,46.0,99.2,0.288,0.011,0.0);
double aCPC12[]={19.25,0.05213,1.197E-5,-1.132E-8};aCPC=aCPC12;gd.input3(1,aCPC);
double aVPC12[]={-6.00435,1.1885,-0.83408,-1.22833};aVPC=aVPC12;gd.input4(1,aVPC);
gd.input5(-74873.0,-50768.0);
double agCH4[][]={{37.17508730836518,-43.772053872440374,-0.08455064288826528,130.74100327363013,298.15,400.0},
{2.308280360899021,97.89435244872931,5.887763951617632,-29.066030387966688,400.0,900.0},
{28.56950123926789,60.59843853981005,-34.06649673774811,-13.956461233222983,900.0,1500.0},
{72.78586849058512,19.714021272164196,-190.2998557041926,-3.2639379592283677,1500.0,2100.0},
{92.44917067621353,6.791019239031948,-326.3141461523196,-0.869405015368204,2100.0,2700.0},
{102.5083961266277,1.7819602099229177,-447.6972203863239,-0.16562371298398668,2700.0,3300.0},
{102.91996766008786,1.621949268991737,-454.8423093235588,-0.1489258923911679,3300.0,3900.0},
{106.2003112847043,0.47297901649692536,-535.2124560322603,-0.035251540174610595,3900.0,4500.0},
{105.92290719765117,0.5352491767734323,-522.1486928989681,-0.03857257521486511,4500.0,5100.0},
{106.90771932394065,0.24249760296751094,-553.0910568428603,-0.014448227994819849,5100.0,6000.0}};
gd.inputCp(agCH4);
double avisiCH4[]={-3.17434898401931,0.455271007474814,-2.73399388607163E-4,8.95312831114117E-8};
double akiCH4[]={3.99296677905716,0.0551053536678452,1.72999763063988E-4,-6.5721336346547E-8};
gd.input_visc( avisiCH4);
gd.input_k(akiCH4);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName13[]={"C","H","O"};atomName=atomName13;double atomN13[]={1.0,4.0,1.0};atomN=atomN13;
gd.input1(13,"CH4O","methanol",atomName,atomN);
gd.input2(32.042,175.5,337.7,512.6,80.9,118.0,0.224,0.556,1.7);
double aCPC13[]={21.15,0.07092,2.587E-5,-2.852E-8};aCPC=aCPC13;gd.input3(1,aCPC);
double aVPC13[]={-8.54796,0.76982,-3.1085,1.54481};aVPC=aVPC13;gd.input4(1,aVPC);
gd.input5(-201300.0,-162600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName14[]={"C","H"};atomName=atomName14;double atomN14[]={2.0,6.0};atomN=atomN14;
gd.input1(14,"C2H6","ethane",atomName,atomN);
gd.input2(30.07,89.9,184.6,305.4,48.8,148.3,0.285,0.099,0.0);
double aCPC14[]={5.409,0.1781,-6.938E-5,8.713E-9};aCPC=aCPC14;gd.input3(1,aCPC);
double aVPC14[]={-6.340307,1.0163,-1.19116,-2.03539};aVPC=aVPC14;gd.input4(1,aVPC);
gd.input5(-84667.0,-32886.0);
double agC2H6[][]={{58.06230921649487,-184.78836690479298,-0.9823798015995937,594.0428912174066,100.0,229.65},
{479.03297239474995,-2364.928195083367,-46.459522456366635,3740.0335370100133,229.65,279.0},
{1101.8358636136104,-4423.888950542867,-177.10277973254944,5274.987327778869,279.0,400.0},
{3.2935178976204496,178.28168304540583,0.8003495795702856,-59.48879344301974,400.0,800.0},
{41.04733014261953,115.75052747650923,-41.09837928220942,-30.083988241380915,800.0,1200.0},
{45.550480453566934,103.85489153567323,-21.960656869080555,-24.220350472439886,1200.0,1500.0},
{154.45024635533528,10.650938188693193,-484.09807796888236,-1.4014184723209353,1500.0,1900.0},
{157.34511955273632,8.655408370323041,-502.2741328681156,-1.0135591638410248,1900.0,2300.0},
{161.24511810951446,6.567413739243016,-542.258147399339,-0.7001067873322487,2300.0,2700.0},
{164.66524100480328,5.056573742023566,-592.2906879405651,-0.5155425299368608,2700.0,3100.0},
{158.53794938763468,7.598553219505648,-485.43097846290044,-0.8136482259540975,3100.0,3500.0},
{164.22191371893103,5.174028982351327,-574.3307145041895,-0.5256820210499236,3500.0,3900.0},
{179.64806027229784,-0.18147176390392877,-956.4713309595865,-0.0015064471598134688,3900.0,4300.0},
{185.56769873721876,-1.9950169231274248,-1145.4879496740782,0.1553831150692342 7,4300.0,4700.0},
{187.21081604436108,-2.585474821073577,-1172.8697129883994,0.21224171557602872,4700.0,5100.0},
{182.68437390457208,-1.7026902071344805,-874.4644076301637,0.16906538548545694,5100.0,5500.0},
{218.71903705995211,-10.645063744571386,-2607.809036864856,0.7931459145437953,5500.0,6000.0}};
gd.inputCp(agC2H6);
double avisiC2H6[]={6.494334947145077,
0.21041244351881475,
6.979895650788042E-4,
-2.133448462416838E-6,
3.242330983865873E-9,
-3.033047705790518E-12,
1.8327337901630014E-15,
-7.16838535477756E-19,
1.7523440075966742E-22,
-2.4331177253737806E-26,
1.4645313953591938E-30};
double akiC2H6[]={3.923490856126888,
-0.051669360489513615,
5.300387662608244E-4,
-7.378002045639982E-7,
7.514433396365195E-10,
-5.687587513247988E-13,
3.009328668405373E-16,
-1.0680298288516747E-19,
2.415814359322047E-23,
-3.14168409538445E-27,
1.7860602324704788E-31};
gd.input_visc( avisiC2H6);
gd.input_k(akiC2H6);
gi.addElement(gd);

gd=new Gas_Data();
String atomName15[]={"C","H"};atomName=atomName15;double atomN15[]={3.0,8.0};atomN=atomN15;
gd.input1(15,"C3H8","propane",atomName,atomN);
gd.input2(44.094,85.5,231.1,369.8,42.5,203.0,0.281,0.153,0.0);
double aCPC15[]={-4.224,0.3063,-1.586E-4,3.215E-8};aCPC=aCPC15;gd.input3(1,aCPC);
double aVPC15[]={-6.72219,1.33236,-2.13868,-1.38551};aVPC=aVPC15;gd.input4(1,aVPC);
gd.input5(-103847.0,-23489.0);
double agC3H8[][]={{-17.455324679189104,327.42434186360583,5.562628862520463,-143.79381263703087,200.0,575.0},
{43.93237921183824,186.3619038411499,-28.904361095303813,-52.73401666231229,575.0,950.0},
{75.27466596237132,141.6676139162145,-72.39627008083784,-35.083204611177905,950.0,1325.0},
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{150.59414337849717,63.53009532639892,-281.99253211380716,-12.210290510455662,1325.0,1700.0},
{190.82007096841596,31.451301269139393,-470.60130108205584,-5.000909027568889,1700.0,2075.0},
{214.74240255099542,15.892025811592456,-638.8650089557747,-2.15082432143284,2075.0,2450.0},
{228.98712873880444,8.062503749873077,-778.9913119619915,-0.9393046198598,2450.0,2825.0},
{237.05494606227614,4.220245902353497,-884.6210547737606,-0.4242863770227898,2825.0,3200.0},
{241.15635138507517,2.495932170649376,-953.4903297995063,-0.22028626938729962,3200.0,3575.0},
{242.93340026942886,1.82712976358739,-990.7127840413975,-0.14946307274629358,3575.0,3950.0},
{243.78450278195191,1.5387771274019881,-1012.7098258168786,-0.12197547953359193,3950.0,4325.0},
{245.02855507379618,1.1570253036532612,-1051.8916836527972,-0.08901804697251668,4325.0,4700.0},
{247.9858284357848,0.3215661199198096,-1161.7631933971995,-0.02261855164634984,4700.0,5075.0},
{254.0333203646043,-1.2626962019283086,-1423.0354468733278,0.0941352033099196,5075.0,5450.0},
{267.912052370946,-4.6252638227761835,-2124.1532593222178,0.3233313964919601,5450.0,6000.0}};
gd.inputCp(agC3H8);
double avisiC3H8[]={10.476238412582333,
0.1312021198776841,
8.235826465107063E-4,
-2.1991065392309257E-6,
3.144431526525468E-9,
-2.828754855521798E-12,
1.6622597667644461E-15,
-6.36647021717235E-19,
1.5310637954908473E-22,
-2.0982901682596035E-26,
1.249629665496125E-30};
//{-54.62,3.2722,-1.0672e-3};
double akiC3H8[]={3.821344207178443,
-0.0575285059979734,
4.700390557836356E-4,
-5.023422673351598E-7,
3.086973538823273E-10,
-1.0409900672911725E-13,
1.6585055762503053E-18,
1.5674578788244127E-20,
-6.80965163648289E-24,
1.270138576338993E-27,
-9.227916039676528E-32};
//{-8.69,6.6409e-2,7.876e5};
gd.input_visc( avisiC3H8);
gd.input_k(akiC3H8);
gi.addElement(gd);

gd=new Gas_Data();
String atomName16[]={"C","H","O"};atomName=atomName16;double atomN16[]={3.0,6.0,1.0};atomN=atomN16;
gd.input1(16,"C3H6O","propionaldehyde",atomName,atomN);
gd.input2(58.08,193.0,321.0,515.3,63.3,0.0,0.0,0.313,2.7);
double aCPC16[]={11.72,0.2614,-1.3E-4,2.126E-8};aCPC=aCPC16;gd.input3(1,aCPC);
double aVPC16[]={-7.18479,1.00298,-1.49247,-5.13288};aVPC=aVPC16;gd.input4(1,aVPC);
gd.input5(-192200.0,-130500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName17[]={"C","H"};atomName=atomName17;double atomN17[]={4.0,10.0};atomN=atomN17;
gd.input1(17,"C4H10","n-butane",atomName,atomN);
gd.input2(58.124,134.8,272.7,425.2,38.0,255.0,0.274,0.199,0.0);
double aCPC17[]={9.487,0.3313,-1.108E-4,-2.822E-9};aCPC=aCPC17;gd.input3(1,aCPC);
double aVPC17[]={-6.88709,1.15157,-1.99873,-3.13003};aVPC=aVPC17;gd.input4(1,aVPC);
gd.input5(-124733.0,-15707.0);
double agC4H10[][]={{-20.879822035641865,430.1502104442387,7.650832781384738,-194.07667102568325,200.0,575.0},
{63.0779637714285,235.6032959012294,-38.85555787975348,-67.26854674022152,575.0,950.0},
{103.69747976338785,177.53060614477718,-94.69626772742187,-44.303770532377435,950.0,1325.0},
{199.5961925343835,77.64959413952538,-359.5166440966679,-14.94944241868323,1325.0,1700.0},
{248.6896301953471,38.49786277514182,-589.6859764158285,-6.150181718983462,1700.0,2075.0},
{277.81674134475765,19.552673553719348,-794.5438056151678,-2.6797556511080023,2075.0,2450.0},
{295.12266556599036,10.040425703061683,-964.7776622472601,-1.2078309997268144,2450.0,2825.0},
{304.9389392797524,5.365781157366884,-1093.3167684678046,-0.5812795882699583,2825.0,3200.0},
{310.0299817963726,3.2262289975963743,-1178.870981633676,-0.32824952090184367,3200.0,3575.0},
{312.47709186628924,2.306730145039822,-1230.2975048817555,-0.23103350361905792,3575.0,3950.0},
{314.07528577163646,1.76653434719419,-1271.7975939503765,-0.17965944512210896,3950.0,4325.0},
{316.53222177684495,1.011845685841562,-1349.0270432327284,-0.11444060965612057,4325.0,4700.0},
{321.5721396469666,-0.41309025316461845,-1535.9868533269057,-0.0011026969010695371,4700.0,5075.0},
{330.9972511123334,-2.8831956118829547,-1942.8541370807266,0.18100872901604834,5075.0,5450.0},
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{351.5123416916953,-7.8550878228629655,-2978.6276371445574,0.5199983597768213,5450.0,6000.0}};
gd.inputCp(agC4H10);
double avisiC4H10[]={12.53424390285022,
0.09222895826828714,
8.079776804482356E-4,
-1.986577929208126E-6,
2.703662714441829E-9,
-2.34784347535656E-12,
1.3434115797493016E-15,
-5.039970631480805E-19,
1.1923154078033366E-22,
-1.612480185510182E-26,
9.49876654116041E-31};
//{-49.46,2.9001,-6.9665e-4};
double akiC4H10[]={4.837183548446356,
-0.05908657824665784,
4.462246377355867E-4,
-5.254059637050542E-7,
4.5411848966672596E-10,
-3.0675843605814195E-13,
1.4507832615773797E-16,
-4.644124117436962E-20,
9.57844920026369E-24,
-1.1492390362668416E-27,
6.09927189481355E-32};
//{-1.82,1.9396e-2,1.3818e-4};
gd.input_visc( avisiC4H10);
gd.input_k(akiC4H10);
gi.addElement(gd);

gd=new Gas_Data();
String atomName18[]={"C","H"};atomName=atomName18;double atomN18[]={4.0,10.0};atomN=atomN18;
gd.input1(18,"C4H10","isobutane",atomName,atomN);
gd.input2(58.124,113.6,261.4,408.2,36.5,263.0,0.283,0.183,0.1);
double aCPC18[]={-1.39,0.3847,-1.846E-4,2.895E-8};aCPC=aCPC18;gd.input3(1,aCPC);
double aVPC18[]={-6.95579,1.5009,-2.52717,-1.49776};aVPC=aVPC18;gd.input4(1,aVPC);
gd.input5(-134600.0,-20900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName19[]={"C","H"};atomName=atomName19;double atomN19[]={5.0,12.0};atomN=atomN19;
gd.input1(19,"C5H12","n-pentane",atomName,atomN);
gd.input2(72.151,143.4,309.2,469.7,33.7,304.0,0.263,0.251,0.0);
double aCPC19[]={-3.626,0.4873,-2.58E-4,5.305E-8};aCPC=aCPC19;gd.input3(1,aCPC);
double aVPC19[]={-7.28936,1.53679,-3.08367,-1.02456};aVPC=aVPC19;gd.input4(1,aVPC);
gd.input5(-146440.0,-8201.0);
double agC5H12[][]={{86.14090234694802,282.5734706400868,-63.70346903313784,-80.9365119887851,575.0,950.0},
{173.26683904829534,172.0307802703151,-227.91599537506545,-40.93213124441803,950.0,1325.0},
{258.4406876777329,84.12079473536514,-467.34808637785693,-15.328853542295601,1325.0,1700.0},
{306.62342662655004,45.694129157102935,-693.2333649523431,-6.692280620508739,1700.0,2075.0},
{335.2260732954842,27.09122334595136,-894.4283273572914,-3.284760969799828,2075.0,2450.0},
{352.45377939585694,17.625065734544574,-1064.0060339762979,-1.8204393362400153,2450.0,2825.0},
{362.7972711563928,12.704444880672805,-1199.734279880342,-1.1615914763738098,2825.0,3200.0},
{369.24950190466745,10.00031566382144,-1308.7722149998974,-0.8426638933036465,3200.0,3575.0},
{374.17635623346683,8.158426040085725,-1413.3754781618277,-0.6489052471332123,3575.0,3950.0},
{379.7103590231169,6.29205717784193,-1557.7076208316132,-0.471804640403573,3950.0,4325.0},
{387.9500441887105,3.7569839864808676,-1815.8719561642276,-0.2523707566814986,4325.0,4700.0},
{401.04877085103715,0.04821246057329526,-2300.385748550535,0.04305071434074059,4700.0,5075.0},
{421.2971429502373,-5.2630855476351925,-3172.952811926648,0.4349780420651342,5075.0,5450.0},
{459.68496988483906,-14.573621205206207,-5108.1605692662315,1.0702720949371436,5450.0,6000.0}};
gd.inputCp(agC5H12);
double avisiC5H12[]={12.70497848022488,
0.0812615984569036,
7.000941598027553E-4,
-1.6061752412207282E-6,
2.067418554680492E-9,
-1.7150262430978467E-12,
9.448862046238017E-16,
-3.434841505091071E-19,
7.913325149674872E-23,
-1.0463925106104517E-26,
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6.046481552872138E-31};
//{-32.02,2.6746,-6.6178e-4};
double akiC5H12[]={3.351911192874566,
-0.042036502694680185,
3.3496950757535985E-4,
-2.1732725250220722E-7,
-6.43854355929012E-11,
2.1497042196152144E-13,
-1.778301474901012E-16,
8.13373053753023E-20,
-2.1839674665099465E-23,
3.2251004486619932E-27,
-2.0258367945313976E-31};
//{-1.82,1.9396e-2,1.3818e-4};
gd.input_visc( avisiC5H12);
gd.input_k(akiC5H12);
gi.addElement(gd);

gd=new Gas_Data();
String atomName20[]={"C","H"};atomName=atomName20;double atomN20[]={6.0,6.0};atomN=atomN20;
gd.input1(20,"C6H6","benzene",atomName,atomN);
gd.input2(78.114,278.7,353.2,562.2,48.9,259.0,0.271,0.212,0.0);
double aCPC20[]={-33.92,0.4739,-3.017E-4,7.13E-8};aCPC=aCPC20;gd.input3(1,aCPC);
double aVPC20[]={-6.98273,1.33213,-2.62863,-3.33399};aVPC=aVPC20;gd.input4(1,aVPC);
gd.input5(82927.0,129658.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName21[]={"C","H"};atomName=atomName21;double atomN21[]={6.0,14.0};atomN=atomN21;
gd.input1(21,"C6H14","n-hexane",atomName,atomN);
gd.input2(86.178,177.8,341.9,507.5,30.1,370.0,0.264,0.299,0.0);
double aCPC21[]={-4.413,0.582,-3.119E-4,6.494E-8};aCPC=aCPC21;gd.input3(1,aCPC);
double aVPC21[]={-7.46765,1.44211,-3.28222,-2.50941};aVPC=aVPC21;gd.input4(1,aVPC);
gd.input5(-167193.0,209);
double agC6H14[][]={{-38.07272907565533,645.1420505772853,12.58794787979993,-289.36650644811306,200.0,575.0},
{100.80182631306556,339.7237495867551,-71.27174997483,-101.99845372468062,575.0,950.0},
{173.96685467919446,225.6283794621939,-149.98315941407571,-53.26139442967823,950.0,1325.0},
{290.2904766433794,110.78824423421936,-503.6734096823533,-21.37781207362136,1325.0,1700.0},
{372.89829720561124,44.70689833763279,-888.5392170931432,-6.481762244536206,1700.0,2075.0},
{410.40016913778436,20.178471808098607,-1149.3039958364343,-1.9640706354065092,2075.0,2450.0},
{421.49136441281723,13.989952739207556,-1255.0533268815948,-0.9923810363293954,2450.0,2825.0},
{417.97511275191124,15.605813484460716,-1205.7390787502068,-1.20119316490034,2825.0,3200.0},
{409.3725849601493,19.195176486926428,-1059.0786987757565,-1.622645327688402,3200.0,3575.0},
{404.7351946862817,20.95392325321237,-963.4908737837198,-1.8102776239003455,3575.0,3950.0},
{413.46003296568716,18.05106629393922,-1197.1418406459304,-1.5385935647848987,3950.0,4325.0},
{445.70503502825335,8.160241600904042,-2213.4671781207458,-0.6850504623177162,4325.0,4700.0},
{512.5805625266694,-10.757040916189556,-4691.774742700846,0.8203737976145621,4700.0,5075.0},
{626.3148781076773,-40.58044903017328,-9596.193676890123,3.0203434591586156,5075.0,5450.0},
{850.6733824827817,-94.98715945778237,-20910.214335646604,6.732110884887747,5450.0,6000.0}};
gd.inputCp(agC6H14);
gi.addElement(gd);

gd=new Gas_Data();
String atomName22[]={"C","Cl","F"};atomName=atomName22;double atomN22[]={1.0,2.0,2.0};atomN=atomN22;
gd.input1(22,"CCl2F2","dichlorodifloromethane",atomName,atomN);
gd.input2(120.914,115.4,245.2,385.0,41.4,216.7,0.28,0.204,0.5);
double aCPC22[]={31.6,0.1782,-1.509E-4,4.342E-8};aCPC=aCPC22;gd.input3(1,aCPC);
double aVPC22[]={-7.01657,1.73224,-2.97909,-0.37723};aVPC=aVPC22;gd.input4(1,aVPC);
gd.input5(-481500.0,-442500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName23[]={"C","H"};atomName=atomName23;double atomN23[]={7.0,16.0};atomN=atomN23;
gd.input1(23,"C7H16","n-heptane",atomName,atomN);
gd.input2(100.205,182.6,371.6,540.3,27.4,27.4,432.0,0.263,0.349);
double aCPC23[]={-5.146,0.6762,-3.651E-4,7.658E-8};aCPC=aCPC23;gd.input3(1,aCPC);
double aVPC23[]={-7.67468,1.37068,-3.5362,-3.20243};aVPC=aVPC23;gd.input4(1,aVPC);
gd.input5(-187820.0,8745.0);
gi.addElement(gd);

gd=new Gas_Data();
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String atomName24[]={"C","H"};atomName=atomName24;double atomN24[]={8.0,10.0};atomN=atomN24;
gd.input1(24,"C8H10","ethylbenzene",atomName,atomN);
gd.input2(106.168,178.2,409.3,617.2,36.0,374.0,0.262,0.302,0.4);
double aCPC24[]={-43.1,0.7072,-4.811E-4,1.301E-7};aCPC=aCPC24;gd.input3(1,aCPC);
double aVPC24[]={-7.48645,1.45488,-3.37538,-2.23048};aVPC=aVPC24;gd.input4(1,aVPC);
gd.input5(29810.0,130700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName25[]={"C","H"};atomName=atomName25;double atomN25[]={8.0,18.0};atomN=atomN25;
gd.input1(25,"C8H18","n-octane",atomName,atomN);
gd.input2(114.232,216.4,398.8,568.8,24.9,492.0,0.259,0.398,0.0);
double aCPC25[]={-6.096,0.7712,-4.195E-4,8.855E-8};aCPC=aCPC25;gd.input3(1,aCPC);
double aVPC25[]={-7.91211,1.38007,-3.80435,-4.50132};aVPC=aVPC25;gd.input4(1,aVPC);
gd.input5(-208447.0,17322.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName26[]={"C","H"};atomName=atomName26;double atomN26[]={9.0,20.0};atomN=atomN26;
gd.input1(26,"C9H20","n-nonane",atomName,atomN);
gd.input2(128.259,219.7,424.0,594.6,22.9,548.0,0.26,0.445,0.0);
double aCPC26[]={-8.347,0.8729,-4.823E-4,1.031E-7};aCPC=aCPC26;gd.input3(1,aCPC);
double aVPC26[]={-8.2448,1.57885,-4.38155,-4.04412};aVPC=aVPC26;gd.input4(1,aVPC);
gd.input5(-229032.0,25857.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName27[]={"C","H"};atomName=atomName27;double atomN27[]={10.0,8.0};atomN=atomN27;
gd.input1(27,"C10H8","naphtalene",atomName,atomN);
gd.input2(128.174,353.5,491.1,748.4,40.5,413.0,0.269,0.302,0.0);
double aCPC27[]={-68.8,0.8499,-6.506E-4,1.981E-7};aCPC=aCPC27;gd.input3(1,aCPC);
double aVPC27[]={-7.85178,2.17172,-3.70504,-4.81238};aVPC=aVPC27;gd.input4(1,aVPC);
gd.input5(151100.0,223700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName28[]={"C","H"};atomName=atomName28;double atomN28[]={11.0,10.0};atomN=atomN28;
gd.input1(28,"C11H10","1-methylnaphtalene",atomName,atomN);
gd.input2(142.201,242.7,517.9,772.0,36.0,462.0,0.234,0.31,0.5);
double aCPC28[]={-64.82,0.9387,-6.942E-4,2.016E-7};aCPC=aCPC28;gd.input3(1,aCPC);
double aVPC28[]={-7.5639,1.19577,-3.38134,-2.86388};aVPC=aVPC28;gd.input4(1,aVPC);
gd.input5(116900.0,217800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName29[]={"C","H"};atomName=atomName29;double atomN29[]={11.0,10.0};atomN=atomN29;
gd.input1(29,"C11H10","2-methylnaphtalene",atomName,atomN);
gd.input2(142.201,307.7,514.3,761.0,35.0,462.0,0.26,0.382,0.4);
double aCPC29[]={-56.52,0.8997,-6.469E-4,1.84E-7};aCPC=aCPC29;gd.input3(1,aCPC);
double aVPC29[]={-8.43595,2.88433,-5.70017,2.50897};aVPC=aVPC29;gd.input4(1,aVPC);
gd.input5(116200.0,216300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName30[]={"C","H"};atomName=atomName30;double atomN30[]={12.0,12.0};atomN=atomN30;
gd.input1(30,"C12H12","1-ethylnaphtalene",atomName,atomN);
gd.input2(156.22,259.0,531.5,774.9,31.4,520.0,0.25,0.4,0.0);
double aCPC30[]={-63.819,1.0396,-8.0E-4,2.0E-7};aCPC=aCPC30;gd.input3(1,aCPC);
double aVPC30[]={0.0,0.0,0.0,0.0};aVPC=aVPC30;gd.input4(4,aVPC);
gd.input5(96719.7,226139.87);
gi.addElement(gd);

gd=new Gas_Data();
String atomName31[]={"C","H"};atomName=atomName31;double atomN31[]={13.0,14.0};atomN=atomN31;
gd.input1(31,"C13H14","1-propylnaphtalene",atomName,atomN);
gd.input2(170.25,265.0,546.0,771.5,27.6,580.0,0.25,0.49,0.0);
double aCPC31[]={-60.235,1.1161,-8.0E-4,2.0E-7};aCPC=aCPC31;gd.input3(1,aCPC);
double aVPC31[]={0.0,0.0,0.0,0.0};aVPC=aVPC31;gd.input4(4,aVPC);
gd.input5(74734.95,232797.2);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName32[]={"C","H"};atomName=atomName32;double atomN32[]={14.0,16.0};atomN=atomN32;
gd.input1(32,"C14H16","1-butylnaphtalene",atomName,atomN);
gd.input2(184.28,253.0,562.6,781.5,25.0,630.0,0.24,0.53,0.0);
double aCPC32[]={15.066,0.8659,4.0E-4,6.0E-8};aCPC=aCPC32;gd.input3(1,aCPC);
double aVPC32[]={0.0,0.0,0.0,0.0};aVPC=aVPC32;gd.input4(4,aVPC);
gd.input5(53091.16,240250.06);
gi.addElement(gd);

gd=new Gas_Data();
String atomName33[]={"C","H"};atomName=atomName33;double atomN33[]={10.0,22.0};atomN=atomN33;
gd.input1(33,"C10H22","n-decane",atomName,atomN);
gd.input2(142.286,243.5,447.3,617.7,21.2,603.0,0.249,0.489,0.0);
double aCPC33[]={-7.913,0.9609,-5.288E-4,1.131E-7};aCPC=aCPC33;gd.input3(1,aCPC);
double aVPC33[]={-8.56523,1.97756,-5.81971,-0.29982};aVPC=aVPC33;gd.input4(1,aVPC);
gd.input5(-249659.0,34434.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName34[]={"C","H"};atomName=atomName34;double atomN34[]={11.0,24.0};atomN=atomN34;
gd.input1(34,"C11H24","n-undecane",atomName,atomN);
gd.input2(156.313,247.6,469.1,638.8,19.7,660.0,0.24,0.535,0.0);
double aCPC34[]={-8.395,1.054,-5.799E-4,1.237E-7};aCPC=aCPC34;gd.input3(1,aCPC);
double aVPC34[]={73.501,9305.8,-8.729,8813.0};aVPC=aVPC34;gd.input4(2,aVPC);
gd.input5(-270286.0,43012.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName35[]={"C","H"};atomName=atomName35;double atomN35[]={12.0,26.0};atomN=atomN35;
gd.input1(35,"C12H26","n-dodecane",atomName,atomN);
gd.input2(170.34,263.6,489.5,658.2,18.2,713.0,0.24,0.575,0.0);
double aCPC35[]={-9.328,1.149,-6.347E-4,1.359E-7};aCPC=aCPC35;gd.input3(1,aCPC);
double aVPC35[]={77.628,10012.5,-9.236,10030.0};aVPC=aVPC35;gd.input4(2,aVPC);
gd.input5(-291100.0,50070.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName36[]={"C","H"};atomName=atomName36;double atomN36[]={13.0,28.0};atomN=atomN36;
gd.input1(36,"C13H28","n-tridecane",atomName,atomN);
gd.input2(184.367,267.8,508.6,676.0,17.2,780.0,0.24,0.619,0.0);
double aCPC36[]={-10.46,1.245,-6.912E-4,1.49E-7};aCPC=aCPC36;gd.input3(1,aCPC);
double aVPC36[]={9.5153,3892.91,-98.93,0.0};aVPC=aVPC36;gd.input4(3,aVPC);
gd.input5(-311700.0,58490.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName37[]={"C","H"};atomName=atomName37;double atomN37[]={14.0,30.0};atomN=atomN37;
gd.input1(37,"C14H30","n-tetradecane",atomName,atomN);
gd.input2(198.394,279.0,526.7,693.0,14.4,830.0,0.23,0.581,0.0);
double aCPC37[]={-10.98,1.338,-7.423E-4,1.598E-7};aCPC=aCPC37;gd.input3(1,aCPC);
double aVPC37[]={84.552,11322.9,-10.07,12500.0};aVPC=aVPC37;gd.input4(2,aVPC);
gd.input5(-332300.0,66860.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName38[]={"C","H"};atomName=atomName38;double atomN38[]={15.0,32.0};atomN=atomN38;
gd.input1(38,"C15H32","n-pentadecane",atomName,atomN);
gd.input2(212.421,283.0,543.8,707.0,15.2,880.0,0.23,0.706,0.0);
double aCPC38[]={-11.92,1.433,-7.972E-4,1.72E-7};aCPC=aCPC38;gd.input3(1,aCPC);
double aVPC38[]={88.38,11995.6,-10.54,13840.0};aVPC=aVPC38;gd.input4(2,aVPC);
gd.input5(-353000.0,75280.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName39[]={"C","H"};atomName=atomName39;double atomN39[]={16.0,34.0};atomN=atomN39;
gd.input1(39,"C16H34","n-hexadecane",atomName,atomN);
gd.input2(226.448,291.0,560.0,722.0,14.1,1030.0,0.24,0.742,0.0);
double aCPC39[]={-13.02,1.529,-8.537E-4,1.85E-7};aCPC=aCPC39;gd.input3(1,aCPC);
double aVPC39[]={89.06,12411.3,-10.58,15200.0};aVPC=aVPC39;gd.input4(2,aVPC);
gd.input5(-373600.0,83740.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName40[]={"C","H"};atomName=atomName40;double atomN40[]={17.0,36.0};atomN=atomN40;
gd.input1(40,"C17H36","n-heptadecane",atomName,atomN);
gd.input2(240.475,295.0,575.2,733.0,13.0,1000.0,0.22,0.77,0.0);
double aCPC40[]={-13.97,1.624,-9.081E-4,1.972E-7};aCPC=aCPC40;gd.input3(1,aCPC);
double aVPC40[]={9.5308,4294.55,-124.0,0.0};aVPC=aVPC40;gd.input4(3,aVPC);
gd.input5(-394200.0,92150.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName41[]={"C","H"};atomName=atomName41;double atomN41[]={18.0,38.0};atomN=atomN41;
gd.input1(41,"C18H38","n-octadecane",atomName,atomN);
gd.input2(254.504,301.3,589.5,748.0,12.0,1190.0,0.25,0.79,0.0);
double aCPC41[]={-14.47,1.717,-9.592E-4,2.078E-7};aCPC=aCPC41;gd.input3(1,aCPC);
double aVPC41[]={9.503,4361.79,-129.9,0.0};aVPC=aVPC41;gd.input4(3,aVPC);
gd.input5(-414800.0,100600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName42[]={"C","H"};atomName=atomName42;double atomN42[]={19.0,40.0};atomN=atomN42;
gd.input1(42,"C19H40","n-nonadecane",atomName,atomN);
gd.input2(268.529,305.0,603.1,756.0,11.1,1130.0,0.21,0.827,0.0);
double aCPC42[]={-15.49,1.812,-0.001015,2.205E-7};aCPC=aCPC42;gd.input3(1,aCPC);
double aVPC42[]={9.5331,4450.44,-135.6,0.0};aVPC=aVPC42;gd.input4(3,aVPC);
gd.input5(-435400.0,109000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName43[]={"C","H"};atomName=atomName43;double atomN43[]={20.0,42.0};atomN=atomN43;
gd.input1(43,"C20H42","n-eicosane",atomName,atomN);
gd.input2(282.556,310.0,617.0,767.0,11.1,1110.0,0.19,0.907,0.0);
double aCPC43[]={-22.38,1.939,-0.001117,2.528E-7};aCPC=aCPC43;gd.input3(1,aCPC);
double aVPC43[]={9.8483,4680.46,-141.1,0.0};aVPC=aVPC43;gd.input4(3,aVPC);
gd.input5(-456100.0,117400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName44[]={"C","H"};atomName=atomName44;double atomN44[]={3.0,6.0};atomN=atomN44;
gd.input1(44,"C3H6","propylene",atomName,atomN);
gd.input2(42.081,87.9,225.5,364.9,46.0,181.0,0.274,0.144,0.4);
double aCPC44[]={3.71,0.2345,-1.16E-4,2.205E-8};aCPC=aCPC44;gd.input3(1,aCPC);
double aVPC44[]={-6.64231,1.21857,-1.81005,-2.48212};aVPC=aVPC44;gd.input4(1,aVPC);
gd.input5(20430.0,62760.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName45[]={"C","H"};atomName=atomName45;double atomN45[]={11.0,16.0};atomN=atomN45;
gd.input1(45,"C11H16","penthylbenzene",atomName,atomN);
gd.input2(148.24,198.0,478.6,679.9,26.0,550.0,0.25,0.44,0.0);
double aCPC45[]={-57.4,1.036,-7.0E-4,2.09E-7};aCPC=aCPC45;gd.input3(1,aCPC);
double aVPC45[]={0.0,0.0,0.0,0.0};aVPC=aVPC45;gd.input4(4,aVPC);
gd.input5(-33780.0,153034.85);
gi.addElement(gd);

gd=new Gas_Data();
String atomName46[]={"C","H"};atomName=atomName46;double atomN46[]={12.0,16.0};atomN=atomN46;
gd.input1(46,"C12H18","hexylbenzene",atomName,atomN);
gd.input2(162.27,212.0,499.3,697.5,23.8,620.0,0.25,0.48,0.0);
double aCPC46[]={-0.9436,0.9028,-5.0E-4,9.0E-8};aCPC=aCPC46;gd.input3(1,aCPC);
double aVPC46[]={0.0,0.0,0.0,0.0};aVPC=aVPC46;gd.input4(4,aVPC);
gd.input5(-55059.0,161450.72);
gi.addElement(gd);

gd=new Gas_Data();
String atomName47[]={"C","H"};atomName=atomName47;double atomN47[]={13.0,20.0};atomN=atomN47;
gd.input1(47,"C13H20","heptylbenzene",atomName,atomN);
gd.input2(176.3,225.0,519.2,713.5,22.0,660.0,0.25,0.53,0.0);
double aCPC47[]={1.5097,0.9848,-5.0E-4,1.0E-7};aCPC=aCPC47;gd.input3(1,aCPC);
double aVPC47[]={0.0,0.0,0.0,0.0};aVPC=aVPC47;gd.input4(4,aVPC);
gd.input5(65819.64,-75700.96);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName48[]={"C","H"};atomName=atomName48;double atomN48[]={13.0,22.0};atomN=atomN48;
gd.input1(48,"C14H22","octylbenzene",atomName,atomN);
gd.input2(190.32,237.0,537.6,728.0,20.4,720.0,0.24,0.58,0.0);
double aCPC48[]={3.7589,1.0683,-6.0E-4,1.0E-7};aCPC=aCPC48;gd.input3(1,aCPC);
double aVPC48[]={0.0,0.0,0.0,0.0};aVPC=aVPC48;gd.input4(4,aVPC);
gd.input5(-96301.0,178324.33);
gi.addElement(gd);

gd=new Gas_Data();
String atomName49[]={"C","H"};atomName=atomName49;double atomN49[]={15.0,22.0};atomN=atomN49;
gd.input1(49,"C15H24","nonylbenzene",atomName,atomN);
gd.input2(204.25,249.0,555.2,741.0,19.0,790.0,0.24,0.63,0.0);
double aCPC49[]={-28.737,1.2932,-8.0E-4,2.0E-7};aCPC=aCPC49;gd.input3(1,aCPC);
double aVPC49[]={0.0,0.0,0.0,0.0};aVPC=aVPC49;gd.input4(4,aVPC);
gd.input5(-116942.91,186698.33);
gi.addElement(gd);

gd=new Gas_Data();
String atomName50[]={"C","H"};atomName=atomName50;double atomN50[]={16.0,26.0};atomN=atomN50;
gd.input1(50,"C16H26","decylbenzene",atomName,atomN);
gd.input2(218.38,259.0,571.1,728.0,20.4,720.0,0.24,0.58,0.0);
double aCPC50[]={9.1501,1.2304,-6.0E-4,1.0E-7};aCPC=aCPC50;gd.input3(1,aCPC);
double aVPC50[]={0.0,0.0,0.0,0.0};aVPC=aVPC50;gd.input4(4,aVPC);
gd.input5(-137584.82,195114.2);
gi.addElement(gd);

gd=new Gas_Data();
String atomName51[]={"C","H"};atomName=atomName51;double atomN51[]={17.0,28.0};atomN=atomN51;
gd.input1(51,"C17H28","undecylbenzene",atomName,atomN);
gd.input2(232.4,268.0,586.4,764.0,16.7,910.0,0.24,0.72,0.0);
double aCPC51[]={-31.624,1.4936,-9.0E-4,2.0E-7};aCPC=aCPC51;gd.input3(1,aCPC);
double aVPC51[]={0.0,0.0,0.0,0.0};aVPC=aVPC51;gd.input4(4,aVPC);
gd.input5(-158184.84,203571.94);
gi.addElement(gd);

gd=new Gas_Data();
String atomName52[]={"C","H"};atomName=atomName52;double atomN52[]={18.0,30.0};atomN=atomN52;
gd.input1(52,"C18H30","dodecylbenzene",atomName,atomN);
gd.input2(246.43,276.0,600.8,774.0,15.8,980.0,0.24,0.77,0.0);
double aCPC52[]={33.664,1.307,-6.0E-4,9.0E-8};aCPC=aCPC52;gd.input3(1,aCPC);
double aVPC52[]={0.0,0.0,0.0,0.0};aVPC=aVPC52;gd.input4(4,aVPC);
gd.input5(-178826.77,211945.94);
gi.addElement(gd);

gd=new Gas_Data();
String atomName53[]={"C","O"};atomName=atomName53;double atomN53[]={1.0,1.0};atomN=atomN53;
gd.input1(53,"CO","carbonmonoxide",atomName,atomN);
gd.input2(28.01,68.1,81.7,132.9,35.0,93.2,0.295,0.066,0.1);
double aCPC53[]={30.87,-0.01285,2.789E-5,-1.272E-8};aCPC=aCPC53;gd.input3(1,aCPC);
double aVPC53[]={-6.20798,1.27885,-1.34533,-2.56842};aVPC=aVPC53;gd.input4(1,aVPC);
double agCO[][]={{29.73376778548717,-4.679766031361607,-0.025529728622553927,9.350538396932045,100.0,400.0},
{23.13005250524206,12.686827249008314,2.5301051722197774,-2.7734663129124684,400.0,800.0},
{25.004926819479063,11.391877095395888,-1.7499780869077555,-3.0410565623527788,800.0,1200.0},
{30.81332874189492,4.920503198802276,-15.578333506985855,-1.0148313675275393,1200.0,1600.0},
{34.58471197952544,1.7224379918748358,-31.291640348666462,-0.249296293415937,1600.0,2000.0},
{36.470916880792515,0.48206651083707286,-43.91748714481847,-0.021748014043914368,2000.0,2400.0},
{52.09699131223591,-7.577039174049389,-216.32980062460013,1.142964479494166,2400.0,2800.0},
{23.571392520258147,6.158008521032203,154.64030947031014,-0.7274690838503632,2800.0,3200.0},
{49.72202304225192,-4.846296524735302,-282.9012269248019,0.5748870547297015,3200.0,3600.0},
{62.82692253799129,-8.847055092892463,-662.6300886944244,0.9011120467806892,3600.0,4000.0},
{53.984482562692094,-5.112058025807606,-551.1745101853712,0.47647764663621667,4000.0,4400.0},
{-14.647137338437295,15.289007144262474,1756.004791020823,-1.2306793850863875,4400.0,4800.0},
{97.11230977282466,-15.74074873757222,-2558.342721449988,1.1959240879273012,4800.0,5200.0},
{77.08680260583158,-9.6076359315616,-2008.6177382155465,0.6818950051159565,5200.0,5600.0},
{207.8224027456623,-39.11043022168717,-9573.170476427164,2.550565527570057,5600.0,6000.0}};
gd.inputCp(agCO);
double avisiCO[]={-10.206932025231346,
0.8505025622180326,
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-0.0011247014578199728,
1.4832545520274912E-6,
-1.4433229137416643E-9,
9.993520878621308E-13,
-4.82460944896371E-16,
1.5797244083517816E-19,
-3.335105570623663E-23,
4.088931479465653E-27,
-2.209471012452592E-31};
//{32.9320014410821,0.540487664029441,-1.94231975194201E-4};
double akiCO[]={-3.140814627706189,
0.14235586748824208,
-2.563105456976829E-4,
4.444023213602694E-7,
-4.885534245727624E-10,
3.692803906267557E-13,
-1.9862139978211864E-16,
7.20108750370189E-20,
-1.6697413120475467E-23,
2.2306664295414717E-27,
-1.303942930616325E-31};
gd.input_visc( avisiCO);
gd.input_k(akiCO);
gd.input5(-110527.0,-137163.0);

gi.addElement(gd);

gd=new Gas_Data();
String atomName54[]={"C","O"};atomName=atomName54;double atomN54[]={1.0,2.0};atomN=atomN54;
gd.input1(54,"CO2","carbondioxide",atomName,atomN);
gd.input2(44.0098,216.592,194.5,304.128,73.8,93.9,0.274,0.239,0.0);
double aCPC54[]={19.8,0.07344,-5.602E-5,1.715E-8};aCPC=aCPC54;gd.input3(1,aCPC);
double aVPC54[]={-6.95626,1.19695,-3.12614,2.299448};aVPC=aVPC54;gd.input4(1,aVPC);
gd.input5(-393522.0,-394389.0);
double agCO2[][]={{18.276706282416832,74.82477157094694,0.38856362687164314,-44.469285173789494,298.15,600.0},
{37.48163407256464,25.37750383533334,-9.564104908722078,-7.59294240291845,600.0,1200.0},
{54.2441495167402,5.688598866114662,-46.68918618060732,-1.0313672317827667,1200.0,1800.0},
{61.95600656165789,0.2133924240182685,-93.57979591701138,0.07705248586505074,1800.0,2400.0},
{64.44414785053367,-0.9348654207303824,-125.98141956149136,0.22105373564026365,2400.0,3000.0},
{54.03437906222963,3.4974045113144783,52.20468173408244,-0.3197326873376619,3000.0,3600.0},
{60.16831618749666,1.0255575960742063,-57.78487799411432,-0.040940477914796894,3600.0,4200.0},
{44.24802864693779,5.756787720823266,475.28309378855755,-0.4361858557540068,4200.0,4800.0},
{27.9758385005928,8.469281789736105,1605.257228378785,-0.5078985005049036,4800.0,5400.0},
{59.80715208813105,0.809939448821011,-10.134673926652594,0.008846836870534143,5400.0,6000.0}};
gd.inputCp(agCO2);
double avisiCO2[]={-1.76629106344796,0.565126210250838,-1.88532276569092E-4,-7.70475550981309E-8,2.30189515042086E-10,-
1.99872708748364E-13,8.45339311929731E-17,-1.70181078916019E-20,1.30133178850726E-24};
double akiCO2[]={-0.486468351507844,0.0201726161151732,2.43958455766759E-4,-6.07514098761129E-7,8.97577413703562E-10,-
7.57474509212984E-13,3.4138182475368E-16,-7.42167095733084E-20,6.10863784559108E-24};
gd.input_visc( avisiCO2);
gd.input_k(akiCO2);
gi.addElement(gd);

gd=new Gas_Data();
String atomName55[]={"C","H"};atomName=atomName55;double atomN55[]={8.0,18.0};atomN=atomN55;
gd.input1(55,"C8H18","2,3,3-trimethylpentane",atomName,atomN);
gd.input2(114.232,172.5,387.9,573.6,28.2,455.0,0.269,0.29,0.0);
double aCPC55[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC55;gd.input3(1,aCPC);
double aVPC55[]={-7.41747,1.42778,-3.19166,-1.81367};aVPC=aVPC55;gd.input4(1,aVPC);
gd.input5(-216600.0,18920.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName56[]={"C","H"};atomName=atomName56;double atomN56[]={8.0,18.0};atomN=atomN56;
gd.input1(56,"C8H18","2,3,4-trimethylpentane",atomName,atomN);
gd.input2(114.232,163.9,386.6,566.4,27.3,461.0,0.267,0.315,0.0);
double aCPC56[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC56;gd.input3(1,aCPC);
double aVPC56[]={-7.62,1.60334,-3.57834,-2.04401};aVPC=aVPC56;gd.input4(1,aVPC);
gd.input5(-217600.0,18920.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName57[]={"C","H"};atomName=atomName57;double atomN57[]={8.0,18.0};atomN=atomN57;
gd.input1(57,"C8H18","2-methyl-3-ethylpentane",atomName,atomN);
gd.input2(114.232,158.2,388.8,567.1,27.0,443.0,0.254,0.33,0.0);
double aCPC57[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC57;gd.input3(1,aCPC);
double aVPC57[]={-7.65393,1.54032,-3.64686,-2.5238};aVPC=aVPC57;gd.input4(1,aVPC);
gd.input5(-211300.0,21270.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName58[]={"C","H"};atomName=atomName58;double atomN58[]={8.0,18.0};atomN=atomN58;
gd.input1(58,"C8H18","3-methyl-3-ethylpentane",atomName,atomN);
gd.input2(114.232,182.3,391.4,576.6,28.1,455.0,0.267,0.303,0.0);
double aCPC58[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC58;gd.input3(1,aCPC);
double aVPC58[]={-7.56484,1.5881,-3.4061,-1.71546};aVPC=aVPC58;gd.input4(1,aVPC);
gd.input5(-215100.0,19930.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName59[]={"C","H","N"};atomName=atomName59;double atomN59[]={6.0,11.0,1.0};atomN=atomN59;
gd.input1(59,"C6H11N","capronitrile",atomName,atomN);
gd.input2(97.161,194.0,436.8,622.0,32.5,0.0,0.0,0.524,3.5);
double aCPC59[]={0.0,0.0,0.0,0.0};aCPC=aCPC59;gd.input3(1,aCPC);
double aVPC59[]={9.7814,3677.63,-60.4,0.0};aVPC=aVPC59;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName62[]={"C","H"};atomName=atomName62;double atomN62[]={6.0,12.0};atomN=atomN62;
gd.input1(62,"C6H12","1-hexene",atomName,atomN);
gd.input2(84.163,133.3,336.6,504.0,31.7,350.0,0.26,0.285,0.4);
double aCPC62[]={-1.746,0.5309,-2.903E-4,6.054E-8};aCPC=aCPC62;gd.input3(1,aCPC);
double aVPC62[]={-7.76467,2.29843,-4.44302,0.89947};aVPC=aVPC62;gd.input4(1,aVPC);
gd.input5(-41700.0,87500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName60[]={"C","H"};atomName=atomName60;double atomN60[]={6.0,12.0};atomN=atomN60;
gd.input1(60,"C6H12","cyclohexane",atomName,atomN);
gd.input2(84.162,279.6,353.8,553.5,40.7,308.0,0.273,0.212,0.3);
double aCPC60[]={-54.54,0.6113,-2.523E-4,1.321E-8};aCPC=aCPC60;gd.input3(1,aCPC);
double aVPC60[]={-6.96009,1.31328,-2.75683,-2.45491};aVPC=aVPC60;gd.input4(1,aVPC);
gd.input5(-123200.0,31780.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName61[]={"C","H"};atomName=atomName61;double atomN61[]={6.0,12.0};atomN=atomN61;
gd.input1(61,"C6H12","methylcyclopentane",atomName,atomN);
gd.input2(84.162,130.7,345.0,532.7,37.8,319.0,0.272,0.231,0.0);
double aCPC61[]={-50.11,0.6381,-3.642E-4,8.014E-8};aCPC=aCPC61;gd.input3(1,aCPC);
double aVPC61[]={-7.15937,1.48017,-2.92482,-1.98377};aVPC=aVPC61;gd.input4(1,aVPC);
gd.input5(-106800.0,35800.0);
gi.addElement(gd);


gd=new Gas_Data();
String atomName63[]={"C","H"};atomName=atomName63;double atomN63[]={6.0,12.0};atomN=atomN63;
gd.input1(63,"C6H12","2-hexene,cis",atomName,atomN);
gd.input2(84.162,132.0,342.0,518.0,32.8,351.0,0.27,0.256,0.0);
double aCPC63[]={-9.81,0.5309,-2.717E-4,4.827E-8};aCPC=aCPC63;gd.input3(1,aCPC);
double aVPC63[]={9.5855,2897.97,-39.3,0.0};aVPC=aVPC63;gd.input4(3,aVPC);
gd.input5(-52380.0,76280.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName64[]={"C","H"};atomName=atomName64;double atomN64[]={6.0,12.0};atomN=atomN64;
gd.input1(64,"C6H12","2-hexene,trans",atomName,atomN);
gd.input2(84.162,140.0,341.0,516.0,32.7,351.0,0.27,0.242,0.0);
double aCPC64[]={-32.92,0.6929,-5.619E-4,2.005E-7};aCPC=aCPC64;gd.input3(1,aCPC);
double aVPC64[]={53.818,5734.51,-6.348,3548.0};aVPC=aVPC64;gd.input4(2,aVPC);
gd.input5(-53930.0,76490.0);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName65[]={"C","H"};atomName=atomName65;double atomN65[]={6.0,12.0};atomN=atomN65;
gd.input1(65,"C6H12","3-hexene,cis",atomName,atomN);
gd.input2(84.162,135.3,339.6,517.0,32.8,350.0,0.27,0.225,0.3);
double aCPC65[]={-21.73,0.5811,-3.362E-4,7.457E-8};aCPC=aCPC65;gd.input3(1,aCPC);
double aVPC65[]={9.2182,2680.52,-48.4,0.0};aVPC=aVPC65;gd.input4(3,aVPC);
gd.input5(-47650.0,83070.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName66[]={"C","H"};atomName=atomName66;double atomN66[]={6.0,12.0};atomN=atomN66;
gd.input1(66,"C6H12","3-hexene,trans",atomName,atomN);
gd.input2(84.162,159.7,340.3,519.9,32.5,350.0,0.26,0.227,0.0);
double aCPC66[]={-4.338,0.551,-3.282E-4,8.047E-8};aCPC=aCPC66;gd.input3(1,aCPC);
double aVPC66[]={9.3086,2718.68,-47.77,0.0};aVPC=aVPC66;gd.input4(3,aVPC);
gd.input5(-54470.0,77670.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName67[]={"C","H"};atomName=atomName67;double atomN67[]={6.0,12.0};atomN=atomN67;
gd.input1(67,"C6H12","2-methyl-2-pentene",atomName,atomN);
gd.input2(84.162,138.1,340.5,518.0,32.8,351.0,0.27,0.229,0.0);
double aCPC67[]={-14.75,0.5669,-3.341E-4,7.963E-8};aCPC=aCPC67;gd.input3(1,aCPC);
double aVPC67[]={9.3221,2725.89,-47.64,0.0};aVPC=aVPC67;gd.input4(3,aVPC);
gd.input5(-66530.0,71260.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName68[]={"C","H"};atomName=atomName68;double atomN68[]={6.0,12.0};atomN=atomN68;
gd.input1(68,"C6H12","3-methyl-2-pentene,cis",atomName,atomN);
gd.input2(84.162,138.3,340.9,518.0,32.8,351.0,0.27,0.269,0.0);
double aCPC68[]={-14.75,0.5669,-3.341E-4,7.963E-8};aCPC=aCPC68;gd.input3(1,aCPC);
double aVPC68[]={9.2922,2731.79,-46.47,0.0};aVPC=aVPC68;gd.input4(3,aVPC);
gd.input5(-62220.0,73270.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName69[]={"C","H"};atomName=atomName69;double atomN69[]={6.0,12.0};atomN=atomN69;
gd.input1(69,"C6H12","3-methyl-2-pentene,trans",atomName,atomN);
gd.input2(84.162,134.7,343.6,521.0,32.9,350.0,0.27,0.207,0.0);
double aCPC69[]={-14.75,0.5669,-3.341E-4,7.963E-8};aCPC=aCPC69;gd.input3(1,aCPC);
double aVPC69[]={9.3282,2750.5,-48.33,0.0};aVPC=aVPC69;gd.input4(3,aVPC);
gd.input5(-63140.0,71340.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName70[]={"C","H"};atomName=atomName70;double atomN70[]={6.0,12.0};atomN=atomN70;
gd.input1(70,"C6H12","4-methyl-2-pentene,cis",atomName,atomN);
gd.input2(84.162,139.0,329.6,490.0,30.4,360.0,0.27,0.29,0.0);
double aCPC70[]={-1.675,0.5376,-3.044E-4,6.753E-8};aCPC=aCPC70;gd.input3(1,aCPC);
double aVPC70[]={9.1325,2580.52,-46.56,0.0};aVPC=aVPC70;gd.input4(3,aVPC);
gd.input5(-57480.0,82190.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName71[]={"C","H"};atomName=atomName71;double atomN71[]={6.0,12.0};atomN=atomN71;
gd.input1(71,"C6H12","4-methyl-2-pentene,trans",atomName,atomN);
gd.input2(84.162,132.0,331.7,493.0,30.4,360.0,0.27,0.29,0.0);
double aCPC71[]={12.63,0.5154,-3.007E-4,7.327E-8};aCPC=aCPC71;gd.input3(1,aCPC);
double aVPC71[]={9.2223,2631.57,-46.0,0.0};aVPC=aVPC71;gd.input4(3,aVPC);
gd.input5(-61500.0,79670.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName72[]={"C","H"};atomName=atomName72;double atomN72[]={6.0,12.0};atomN=atomN72;
gd.input1(72,"C6H12","2,3-dimethyl-1-butene",atomName,atomN);
gd.input2(84.162,115.9,328.8,501.0,32.4,343.0,0.27,0.221,0.0);
double aCPC72[]={7.025,0.5585,-3.696E-4,1.063E-7};aCPC=aCPC72;gd.input3(1,aCPC);
double aVPC72[]={9.181,2612.69,-43.78,0.0};aVPC=aVPC72;gd.input4(3,aVPC);
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gd.input5(-66360.0,79090.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName73[]={"C","H"};atomName=atomName73;double atomN73[]={6.0,12.0};atomN=atomN73;
gd.input1(73,"C6H12","2,3-dimethyl-2-butene",atomName,atomN);
gd.input2(84.162,198.9,364.4,524.0,33.6,351.0,0.27,0.239,0.0);
double aCPC73[]={2.294,0.4827,-2.199E-4,3.042E-8};aCPC=aCPC73;gd.input3(1,aCPC);
double aVPC73[]={-7.15852,1.36868,-4.1289,1.53046};aVPC=aVPC73;gd.input4(1,aVPC);
gd.input5(-69840.0,75910.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName74[]={"C","H"};atomName=atomName74;double atomN74[]={6.0,12.0};atomN=atomN74;
gd.input1(74,"C6H12","3,3-dimethyl-1-butene",atomName,atomN);
gd.input2(84.162,158.0,314.4,490.0,32.5,340.0,0.27,0.121,0.0);
double aCPC74[]={-12.56,0.5485,-2.915E-4,5.208E-8};aCPC=aCPC74;gd.input3(1,aCPC);
double aVPC74[]={-6.54633,1.50412,-4.54855,2.96466};aVPC=aVPC74;gd.input4(1,aVPC);
gd.input5(-61550.0,98220.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName75[]={"C","H","O"};atomName=atomName75;double atomN75[]={6.0,12.0,1.0};atomN=atomN75;
gd.input1(75,"C6H12O","cyclohexanol",atomName,atomN);
gd.input2(100.16,298.0,434.3,625.0,37.5,0.0,0.0,0.528,1.7);
double aCPC75[]={-55.53,0.7214,-4.086E-4,8.235E-8};aCPC=aCPC75;gd.input3(1,aCPC);
double aVPC75[]={-8.77758,3.11622,-12.3555,7.5061};aVPC=aVPC75;gd.input4(1,aVPC);
gd.input5(-294800.0,-118000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName76[]={"C","H","O"};atomName=atomName76;double atomN76[]={6.0,12.0,1.0};atomN=atomN76;
gd.input1(76,"C6H12O","ethylpropylketone",atomName,atomN);
gd.input2(100.16,0.0,396.6,582.8,33.2,0.0,0.0,0.378,0.0);
double aCPC76[]={0.0,0.0,0.0,0.0};aCPC=aCPC76;gd.input3(1,aCPC);
double aVPC76[]={9.5,3144.85,-65.19,0.0};aVPC=aVPC76;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName77[]={"C","H","O"};atomName=atomName77;double atomN77[]={6.0,12.0,1.0};atomN=atomN77;
gd.input1(77,"C6H12O","methylisobutylketone",atomName,atomN);
gd.input2(100.16,189.0,389.6,571.0,32.7,0.0,0.0,0.385,2.8);
double aCPC77[]={3.894,0.5656,-3.318E-4,8.231E-8};aCPC=aCPC77;gd.input3(1,aCPC);
double aVPC77[]={-8.54349,2.92801,-5.27311,-2.54507};aVPC=aVPC77;gd.input4(1,aVPC);
gd.input5(-284000.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName78[]={"C","H","O"};atomName=atomName78;double atomN78[]={6.0,12.0,2.0};atomN=atomN78;
gd.input1(78,"C6H12O2","n-butylacetate",atomName,atomN);
gd.input2(116.16,199.7,399.3,579.0,31.4,400.0,0.26,0.417,1.8);
double aCPC78[]={13.62,0.5489,-2.278E-4,7.91E-10};aCPC=aCPC78;gd.input3(1,aCPC);
double aVPC78[]={-8.36658,2.40985,-6.42511,4.85939};aVPC=aVPC78;gd.input4(1,aVPC);
gd.input5(-486800.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName79[]={"C","H","O"};atomName=atomName79;double atomN79[]={6.0,12.0,2.0};atomN=atomN79;
gd.input1(79,"C6H12O2","isobutylacetate",atomName,atomN);
gd.input2(116.16,174.3,389.7,564.0,30.2,414.0,0.267,0.455,1.9);
double aCPC79[]={7.31,0.574,-2.576E-4,1.101E-8};aCPC=aCPC79;gd.input3(1,aCPC);
double aVPC79[]={-8.12456,1.66934,-4.20511,-3.72813};aVPC=aVPC79;gd.input4(1,aVPC);
gd.input5(-495500.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName80[]={"C","H","O"};atomName=atomName80;double atomN80[]={6.0,12.0,2.0};atomN=atomN80;
gd.input1(80,"C6H12O2","ethylbutyrate",atomName,atomN);
gd.input2(116.16,180.0,394.7,569.0,29.6,421.0,0.263,0.461,1.8);
double aCPC80[]={21.51,0.4928,-1.938E-4,3.559E-9};aCPC=aCPC80;gd.input3(1,aCPC);
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double aVPC80[]={-8.00073,1.34045,-3.99843,-3.74347};aVPC=aVPC80;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName81[]={"C","H","O"};atomName=atomName81;double atomN81[]={6.0,12.0,2.0};atomN=atomN81;
gd.input1(81,"C6H12O2","ethylisobutyrate",atomName,atomN);
gd.input2(116.16,185.0,383.2,555.0,29.7,421.0,0.271,0.431,2.1);
double aCPC81[]={0.0,0.0,0.0,0.0};aCPC=aCPC81;gd.input3(1,aCPC);
double aVPC81[]={-8.08582,1.61436,-4.14816,-3.8072};aVPC=aVPC81;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName82[]={"C","H","O"};atomName=atomName82;double atomN82[]={6.0,12.0,2.0};atomN=atomN82;
gd.input1(82,"C6H12O2","n-propylpropionate",atomName,atomN);
gd.input2(116.16,197.3,395.8,571.0,30.2,0.0,0.0,0.0,1.8);
double aCPC82[]={0.0,0.0,0.0,0.0};aCPC=aCPC82;gd.input3(1,aCPC);
double aVPC82[]={-8.00913,1.33297,-3.97513,-3.83674};aVPC=aVPC82;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName83[]={"C","H"};atomName=atomName83;double atomN83[]={6.0,14.0};atomN=atomN83;
gd.input1(83,"C6H14","2-methylpentane",atomName,atomN);
gd.input2(86.178,119.5,333.4,497.5,30.1,367.0,0.267,0.278,0.0);
double aCPC83[]={-10.57,0.6184,-3.573E-4,8.058E-8};aCPC=aCPC83;gd.input3(1,aCPC);
double aVPC83[]={-7.31728,1.3394,-3.06807,-1.99255};aVPC=aVPC83;gd.input4(1,aVPC);
gd.input5(-174400.0,-5020.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName84[]={"C","H"};atomName=atomName84;double atomN84[]={6.0,14.0};atomN=atomN84;
gd.input1(84,"C6H14","3-methylpentane",atomName,atomN);
gd.input2(86.178,155.0,336.4,504.5,31.2,367.0,0.273,0.272,0.0);
double aCPC84[]={-2.386,0.569,-2.87E-4,5.033E-8};aCPC=aCPC84;gd.input3(1,aCPC);
double aVPC84[]={-7.27084,1.26113,-2.81741,-2.17642};aVPC=aVPC84;gd.input4(1,aVPC);
gd.input5(-171700.0,-2140.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName85[]={"C","H"};atomName=atomName85;double atomN85[]={6.0,14.0};atomN=atomN85;
gd.input1(85,"C6H14","2,2-dimethylbutane",atomName,atomN);
gd.input2(86.178,173.3,322.8,488.8,30.8,359.0,0.272,0.232,0.0);
double aCPC85[]={-16.63,0.6293,-3.481E-4,6.85E-8};aCPC=aCPC85;gd.input3(1,aCPC);
double aVPC85[]={-7.24296,1.66876,-3.23718,-0.53171};aVPC=aVPC85;gd.input4(1,aVPC);
gd.input5(-185700.0,-9630.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName86[]={"C","H"};atomName=atomName86;double atomN86[]={6.0,14.0};atomN=atomN86;
gd.input1(86,"C6H14","2,3-dimethylbutane",atomName,atomN);
gd.input2(86.178,144.6,331.1,500.0,31.3,358.0,0.269,0.247,0.0);
double aCPC86[]={-14.61,0.615,-3.376E-4,6.82E-8};aCPC=aCPC86;gd.input3(1,aCPC);
double aVPC86[]={-7.2787,1.56349,-3.05387,-1.57752};aVPC=aVPC86;gd.input4(1,aVPC);
gd.input5(-177900.0,-4100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName87[]={"C","H","O"};atomName=atomName87;double atomN87[]={6.0,14.0,1.0};atomN=atomN87;
gd.input1(87,"C6H14O","1-hexanol",atomName,atomN);
gd.input2(102.177,229.2,430.2,611.0,40.5,381.0,0.3,0.56,1.8);
double aCPC87[]={4.811,0.5891,-3.01E-4,5.426E-8};aCPC=aCPC87;gd.input3(1,aCPC);
double aVPC87[]={11.4792,4055.45,-76.49,0.0};aVPC=aVPC87;gd.input4(3,aVPC);
gd.input5(-317800.0,-135700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName88[]={"C","H","O"};atomName=atomName88;double atomN88[]={6.0,14.0,1.0};atomN=atomN88;
gd.input1(88,"C6H14O","ethylbutylether",atomName,atomN);
gd.input2(102.177,170.0,365.4,531.0,30.4,390.0,0.27,0.4,1.2);
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double aCPC88[]={23.63,0.5367,-2.528E-4,4.157E-8};aCPC=aCPC88;gd.input3(1,aCPC);
double aVPC88[]={-8.30292,2.02889,-3.26245,-6.32274};aVPC=aVPC88;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName89[]={"C","H","O"};atomName=atomName89;double atomN89[]={6.0,14.0,1.0};atomN=atomN89;
gd.input1(89,"C6H14O","dipropylether",atomName,atomN);
gd.input2(102.177,151.0,363.2,530.6,30.3,0.0,0.0,0.369,1.2);
double aCPC89[]={18.62,0.5335,-2.285E-4,2.442E-8};aCPC=aCPC89;gd.input3(1,aCPC);
double aVPC89[]={-8.22229,2.2211,-3.26245,-6.32274};aVPC=aVPC89;gd.input4(1,aVPC);
gd.input5(-293100.0,-105600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName90[]={"C","H","O"};atomName=atomName90;double atomN90[]={6.0,14.0,1.0};atomN=atomN90;
gd.input1(90,"C6H14O","diisopropylether",atomName,atomN);
gd.input2(102.177,187.7,341.7,500.3,28.8,386.0,0.262,0.331,1.2);
double aCPC90[]={7.505,0.5849,-3.027E-4,5.845E-8};aCPC=aCPC90;gd.input3(1,aCPC);
double aVPC90[]={-7.62613,1.29308,-2.90101,-6.14467};aVPC=aVPC90;gd.input4(1,aVPC);
gd.input5(-319000.0,122000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName91[]={"C","H","N"};atomName=atomName91;double atomN91[]={6.0,15.0,1.0};atomN=atomN91;
gd.input1(91,"C6H15N","dipropylamine",atomName,atomN);
gd.input2(101.193,233.6,382.5,555.8,29.9,0.0,0.0,0.471,1.0);
double aCPC91[]={6.46,0.6293,-3.39E-4,7.072E-8};aCPC=aCPC91;gd.input3(1,aCPC);
double aVPC91[]={-8.56471,2.93461,-5.56089,0.56571};aVPC=aVPC91;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName92[]={"C","H","N"};atomName=atomName92;double atomN92[]={6.0,15.0,1.0};atomN=atomN92;
gd.input1(92,"C6H15N","diisopropylamine",atomName,atomN);
gd.input2(101.193,212.2,357.1,523.1,30.2,0.0,0.0,0.36,1.0);
double aCPC92[]={0.0,0.0,0.0,0.0};aCPC=aCPC92;gd.input3(1,aCPC);
double aVPC92[]={-7.84319,1.80097,-4.66457,-0.29364};aVPC=aVPC92;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName93[]={"C","H","N"};atomName=atomName93;double atomN93[]={6.0,15.0,1.0};atomN=atomN93;
gd.input1(93,"C6H15N","triethylamine",atomName,atomN);
gd.input2(101.193,158.4,362.5,535.0,30.3,389.0,0.265,0.32,0.9);
double aCPC93[]={-18.43,0.7155,-4.392E-4,1.092E-7};aCPC=aCPC93;gd.input3(1,aCPC);
double aVPC93[]={-11.3617,10.0092,-13.475,-9.36035};aVPC=aVPC93;gd.input4(1,aVPC);
gd.input5(-99650.0,110400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName94[]={"C","F"};atomName=atomName94;double atomN94[]={7.0,14.0};atomN=atomN94;
gd.input1(94,"C7F14","perfluoromethylcyclohexane",atomName,atomN);
gd.input2(350.055,0.0,349.5,486.8,23.3,0.0,0.0,0.491,0.0);
double aCPC94[]={0.0,0.0,0.0,0.0};aCPC=aCPC94;gd.input3(1,aCPC);
double aVPC94[]={-10.5469,6.38028,-10.694,11.6006};aVPC=aVPC94;gd.input4(1,aVPC);
gd.input5(-2898000.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName95[]={"C","F"};atomName=atomName95;double atomN95[]={7.0,16.0};atomN=atomN95;
gd.input1(95,"C7F16","perfluoro-n-heptane",atomName,atomN);
gd.input2(388.051,195.0,355.6,474.8,16.2,664.0,0.273,0.556,0.0);
double aCPC95[]={0.0,0.0,0.0,0.0};aCPC=aCPC95;gd.input3(1,aCPC);
double aVPC95[]={-9.13392,2.75328,-8.33813,6.82085};aVPC=aVPC95;gd.input4(1,aVPC);
gd.input5(-3387000.0,-3089000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName96[]={"C","H","F"};atomName=atomName96;double atomN96[]={7.0,3.0,5.0};atomN=atomN96;
gd.input1(96,"C7H3F5","2,3,4,5,6-pentafluorotoluene",atomName,atomN);
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gd.input2(182.091,0.0,390.7,566.5,31.3,384.0,0.255,0.415,0.0);
double aCPC96[]={0.0,0.0,0.0,0.0};aCPC=aCPC96;gd.input3(1,aCPC);
double aVPC96[]={-8.05688,1.46673,-3.82439,-2.78727};aVPC=aVPC96;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName97[]={"C","H","N"};atomName=atomName97;double atomN97[]={7.0,5.0,1.0};atomN=atomN97;
gd.input1(97,"C7H5N","benzonitrile",atomName,atomN);
gd.input2(103.124,260.0,464.3,699.4,42.2,0.0,0.0,0.362,3.5);
double aCPC97[]={-26.05,0.5732,-4.43E-4,1.349E-7};aCPC=aCPC97;gd.input3(1,aCPC);
double aVPC97[]={53.154,7912.31,-5.881,4898.0};aVPC=aVPC97;gd.input4(2,aVPC);
gd.input5(219000.0,261000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName98[]={"C","H","O"};atomName=atomName98;double atomN98[]={7.0,6.0,1.0};atomN=atomN98;
gd.input1(98,"C7H6O","benzaldehyde",atomName,atomN);
gd.input2(106.124,216.0,452.2,694.8,45.4,0.0,0.0,0.316,2.8);
double aCPC98[]={-12.14,0.4961,-2.845E-4,5.167E-8};aCPC=aCPC98;gd.input3(1,aCPC);
double aVPC98[]={-7.16527,0.5271,-1.51484,-7.92908};aVPC=aVPC98;gd.input4(1,aVPC);
gd.input5(-36800.0,22400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName99[]={"C","H","O"};atomName=atomName99;double atomN99[]={7.0,6.0,2.0};atomN=atomN99;
gd.input1(99,"C7H6O2","benzoicacid",atomName,atomN);
gd.input2(122.124,395.6,523.0,752.0,45.6,341.0,0.25,0.62,1.7);
double aCPC99[]={-51.29,0.6293,-4.237E-4,1.062E-7};aCPC=aCPC99;gd.input3(1,aCPC);
double aVPC99[]={10.5432,4190.7,125.2,0.0};aVPC=aVPC99;gd.input4(3,aVPC);
gd.input5(-290400.0,-210600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName100[]={"C","H"};atomName=atomName100;double atomN100[]={7.0,8.0};atomN=atomN100;
gd.input1(100,"C7H8","toluene",atomName,atomN);
gd.input2(92.141,178.0,383.8,591.8,41.0,316.0,0.263,0.263,0.4);
double aCPC100[]={-24.35,0.5125,-2.765E-4,4.911E-8};aCPC=aCPC100;gd.input3(1,aCPC);
double aVPC100[]={-7.28607,1.38091,-2.83433,-2.79168};aVPC=aVPC100;gd.input4(1,aVPC);
gd.input5(50030.0,122100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName101[]={"C","H","O"};atomName=atomName101;double atomN101[]={7.0,8.0,1.0};atomN=atomN101;
gd.input1(101,"C7H8O","methylphenylether",atomName,atomN);
gd.input2(108.14,235.7,426.8,645.6,42.5,0.0,0.0,0.347,1.2);
double aCPC101[]={0.0,0.0,0.0,0.0};aCPC=aCPC101;gd.input3(1,aCPC);
double aVPC101[]={-7.87545,1.83291,-4.06977,-2.18906};aVPC=aVPC101;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName102[]={"C","H","O"};atomName=atomName102;double atomN102[]={7.0,8.0,1.0};atomN=atomN102;
gd.input1(102,"C7H8O","benzylalcohol",atomName,atomN);
gd.input2(108.14,257.8,478.6,720.2,44.0,0.0,0.0,0.0,1.7);
double aCPC102[]={-7.398,0.5481,-3.357E-4,7.771E-8};aCPC=aCPC102;gd.input3(1,aCPC);
double aVPC102[]={-7.09506,1.18389,-9.14255,5.56311};aVPC=aVPC102;gd.input4(1,aVPC);
gd.input5(-94080.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName103[]={"C","H","O"};atomName=atomName103;double atomN103[]={7.0,8.0,1.0};atomN=atomN103;
gd.input1(103,"C7H8O","o-cresol",atomName,atomN);
gd.input2(108.14,304.1,464.2,697.6,50.1,0.0,0.0,0.433,1.6);
double aCPC103[]={-32.28,0.7055,-5.924E-4,2.124E-7};aCPC=aCPC103;gd.input3(1,aCPC);
double aVPC103[]={-8.82061,3.14917,-6.63041,-0.84857};aVPC=aVPC103;gd.input4(1,aVPC);
gd.input5(-128700.0,-33000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName104[]={"C","H","O"};atomName=atomName104;double atomN104[]={7.0,8.0,1.0};atomN=atomN104;
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```
gd.input1(104,"C7H8O","m-cresol",atomName,atomN);
gd.input2(108.14,285.4,475.4,705.8,45.6,309.0,0.24,0.454,1.8);
double aCPC104[]={-45.01,0.7264,-6.029E-4,2.077E-7};aCPC=aCPC104;gd.input3(1,aCPC);
double aVPC104[]={-8.58506,2.82624,-8.57418,8.74822};aVPC=aVPC104;gd.input4(1,aVPC);
gd.input5(-132400.0,-40570.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName105[]={"C","H","O"};atomName=atomName105;double atomN105[]={7.0,8.0,1.0};atomN=atomN105;
gd.input1(105,"C7H8O","p-cresol",atomName,atomN);
gd.input2(108.14,307.9,475.1,704.6,51.5,0.0,0.0,0.505,1.6);
double aCPC105[]={-40.63,0.7055,-5.757E-4,1.967E-7};aCPC=aCPC105;gd.input3(1,aCPC);
double aVPC105[]={-9.23951,3.2988,-7.17725,-0.48};aVPC=aVPC105;gd.input4(1,aVPC);
gd.input5(-125500.0,-30900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName106[]={"C","H","N"};atomName=atomName106;double atomN106[]={7.0,9.0,1.0};atomN=atomN106;
gd.input1(106,"C7H9N","n-methylaniline",atomName,atomN);
gd.input2(107.156,216.0,469.4,701.0,52.0,0.0,0.0,0.475,1.7);
double aCPC106[]={0.0,0.0,0.0,0.0};aCPC=aCPC106;gd.input3(1,aCPC);
double aVPC106[]={9.6864,3756.28,-80.71,0.0};aVPC=aVPC106;gd.input4(3,aVPC);
gd.input5(85410.0,199300.0);
gi.addElement(gd);
}
  public void data2()
  {Gas_Data gd=new Gas_Data();
String atomName107[]={"C","H","N"};atomName=atomName107;double atomN107[]={7.0,9.0,1.0};atomN=atomN107;
gd.input1(107,"C7H9N","o-toluidine",atomName,atomN);
gd.input2(107.156,258.4,473.5,694.0,37.5,0.0,0.0,0.438,1.6);
double aCPC107[]={0.0,0.0,0.0,0.0};aCPC=aCPC107;gd.input3(1,aCPC);
double aVPC107[]={-8.68458,2.72553,-5.9462,-1.09185};aVPC=aVPC107;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName108[]={"C","H","N"};atomName=atomName108;double atomN108[]={7.0,9.0,1.0};atomN=atomN108;
gd.input1(108,"C7H9N","m-toluidine",atomName,atomN);
gd.input2(107.156,242.8,476.6,709.0,41.5,0.0,0.0,0.41,1.5);
double aCPC108[]={-15.99,0.5681,-3.033E-4,4.643E-8};aCPC=aCPC108;gd.input3(1,aCPC);
double aVPC108[]={-8.43741,2.58101,-6.00776,-1.52856};aVPC=aVPC108;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName109[]={"C","H"};atomName=atomName109;double atomN109[]={7.0,14.0};atomN=atomN109;
gd.input1(109,"C7H14","cycloheptane",atomName,atomN);
gd.input2(98.189,265.0,391.6,604.2,38.1,353.0,0.268,0.237,0.0);
double aCPC109[]={-76.19,0.7867,-4.204E-4,7.561E-8};aCPC=aCPC109;gd.input3(1,aCPC);
double aVPC109[]={9.1616,3066.05,-56.8,0.0};aVPC=aVPC109;gd.input4(3,aVPC);
gd.input5(-119400.0,63050.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName110[]={"C","H"};atomName=atomName110;double atomN110[]={7.0,14.0};atomN=atomN110;
gd.input1(110,"C7H14","1,1-dimethylcyclopentane",atomName,atomN);
gd.input2(98.189,203.4,361.0,547.0,34.4,360.0,0.27,0.273,0.0);
double aCPC110[]={-57.89,0.767,-4.501E-4,1.01E-7};aCPC=aCPC110;gd.input3(1,aCPC);
double aVPC110[]={-7.56029,1.82906,-2.90303,-3.86394};aVPC=aVPC110;gd.input4(1,aVPC);
gd.input5(-138400.0,39060.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName111[]={"C","H"};atomName=atomName111;double atomN111[]={7.0,14.0};atomN=atomN111;
gd.input1(111,"C7H14","1,2-dimethylcyclopentane-cis",atomName,atomN);
gd.input2(98.189,219.3,372.7,564.8,34.4,368.0,0.27,0.269,0.0);
double aCPC111[]={-55.64,0.7616,-0.4484,1.014E-7};aCPC=aCPC111;gd.input3(1,aCPC);
double aVPC111[]={-7.67242,2.2016,-3.86394,-1.16796};aVPC=aVPC111;gd.input4(1,aVPC);
gd.input5(-129600.0,45760.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName112[]={"C","H"};atomName=atomName112;double atomN112[]={7.0,14.0};atomN=atomN112;
gd.input1(112,"C7H14","1,2-dimethylcyclopentane-trans",atomName,atomN);
gd.input2(98.189,155.6,365.0,553.2,34.4,362.0,0.27,0.269,0.0);
double aCPC112[]={-54.52,0.7591,-4.48E-4,1.017E-7};aCPC=aCPC112;gd.input3(1,aCPC);
double aVPC112[]={-7.19675,1.03696,-1.93618,-5.30531};aVPC=aVPC112;gd.input4(1,aVPC);
gd.input5(-136800.0,38390.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName113[]={"C","H"};atomName=atomName113;double atomN113[]={7.0,14.0};atomN=atomN113;
gd.input1(113,"C7H14","ethylcyclopentane",atomName,atomN);
gd.input2(98.189,134.7,376.6,569.5,34.0,375.0,0.269,0.271,0.0);
double aCPC113[]={-55.31,0.7511,-4.396E-4,1.004E-7};aCPC=aCPC113;gd.input3(1,aCPC);
double aVPC113[]={-7.68089,2.28014,-4.40365,0.54338};aVPC=aVPC113;gd.input4(1,aVPC);
gd.input5(-127200.0,44590.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName114[]={"C","H"};atomName=atomName114;double atomN114[]={7.0,14.0};atomN=atomN114;
gd.input1(114,"C7H14","methylcyclohexane",atomName,atomN);
gd.input2(98.189,146.6,374.1,572.2,34.7,368.0,0.268,0.236,0.0);
double aCPC114[]={-61.92,0.7842,-4.438E-4,9.366E-8};aCPC=aCPC114;gd.input3(1,aCPC);
double aVPC114[]={-7.01915,1.09615,-2.37009,-3.37562};aVPC=aVPC114;gd.input4(1,aVPC);
gd.input5(-154900.0,27300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName115[]={"C","H"};atomName=atomName115;double atomN115[]={7.0,14.0};atomN=atomN115;
gd.input1(115,"C7H14","1-heptene",atomName,atomN);
gd.input2(98.189,154.3,366.8,537.3,28.3,440.0,0.28,0.358,0.3);
double aCPC115[]={-3.303,0.6297,-3.512E-4,7.607E-8};aCPC=aCPC115;gd.input3(1,aCPC);
double aVPC115[]={-8.26875,3.02688,-6.18709,4.33049};aVPC=aVPC115;gd.input4(1,aVPC);
gd.input5(-62340.0,95880.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName116[]={"C","H"};atomName=atomName116;double atomN116[]={7.0,14.0};atomN=atomN116;
gd.input1(116,"C7H14","2,3,3-trimethyl-1-butene",atomName,atomN);
gd.input2(98.189,163.3,351.0,533.0,28.9,400.0,0.26,0.192,0.0);
double aCPC116[]={0.0,0.0,0.0,0.0};aCPC=aCPC116;gd.input3(1,aCPC);
double aVPC116[]={9.0334,2719.47,-49.56,0.0};aVPC=aVPC116;gd.input4(3,aVPC);
gd.input5(-86540.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName117[]={"C","H","O"};atomName=atomName117;double atomN117[]={7.0,14.0,2.0};atomN=atomN117;
gd.input1(117,"C7H14O2","n-propylbutyrate",atomName,atomN);
gd.input2(130.187,176.0,416.2,590.0,27.1,0.0,0.0,0.0,1.8);
double aCPC117[]={0.0,0.0,0.0,0.0};aCPC=aCPC117;gd.input3(1,aCPC);
double aVPC117[]={-8.28062,1.40511,-4.19323,-3.70158};aVPC=aVPC117;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName118[]={"C","H","O"};atomName=atomName118;double atomN118[]={7.0,14.0,2.0};atomN=atomN118;
gd.input1(118,"C7H14O2","n-propylisobutyrate",atomName,atomN);
gd.input2(130.187,0.0,408.6,581.0,28.3,0.0,0.0,0.0,0.0);
double aCPC118[]={0.0,0.0,0.0,0.0};aCPC=aCPC118;gd.input3(1,aCPC);
double aVPC118[]={-8.52052,2.1066,-4.44053,-3.9042};aVPC=aVPC118;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName119[]={"C","H","O"};atomName=atomName119;double atomN119[]={7.0,14.0,2.0};atomN=atomN119;
gd.input1(119,"C7H14O2","isobutylpropionate",atomName,atomN);
gd.input2(130.187,201.8,410.0,583.0,27.7,0.0,0.0,0.0,0.0);
double aCPC119[]={0.0,0.0,0.0,0.0};aCPC=aCPC119;gd.input3(1,aCPC);
double aVPC119[]={-8.32761,1.56574,-3.97739,-4.71845};aVPC=aVPC119;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName120[]={"C","H"};atomName=atomName120;double atomN120[]={7.0,16.0};atomN=atomN120;
gd.input1(120,"C7H16","3-methylhexane",atomName,atomN);
gd.input2(100.205,100.0,365.0,535.3,28.1,404.0,0.255,0.323,0.0);
double aCPC120[]={-7.046,0.6837,-3.734E-4,7.834E-8};aCPC=aCPC120;gd.input3(1,aCPC);
double aVPC120[]={-7.58592,1.47394,-3.52511,-2.35419};aVPC=aVPC120;gd.input4(1,aVPC);
gd.input5(-192400.0,4600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName121[]={"C","H"};atomName=atomName121;double atomN121[]={7.0,16.0};atomN=atomN121;
gd.input1(121,"C7H16","2,2-dimethylpentane",atomName,atomN);
gd.input2(100.205,149.4,352.4,520.5,27.7,416.0,0.266,0.287,0.0);
double aCPC121[]={-50.1,0.8956,-6.36E-4,1.736E-7};aCPC=aCPC121;gd.input3(1,aCPC);
double aVPC121[]={-7.45564,1.56232,-3.4462,-1.80802};aVPC=aVPC121;gd.input4(1,aVPC);
gd.input5(-206300.0,840.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName122[]={"C","H"};atomName=atomName122;double atomN122[]={7.0,16.0};atomN=atomN122;
gd.input1(122,"C7H16","2,3-dimethylpentane",atomName,atomN);
gd.input2(100.205,0.0,362.9,537.4,29.1,393.0,0.256,0.296,0.0);
double aCPC122[]={-7.046,0.6837,-3.734E-4,7.834E-8};aCPC=aCPC122;gd.input3(1,aCPC);
double aVPC122[]={-7.46078,1.47778,-3.37079,-1.88997};aVPC=aVPC122;gd.input4(1,aVPC);
gd.input5(-199400.0,670.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName123[]={"C","H"};atomName=atomName123;double atomN123[]={7.0,16.0};atomN=atomN123;
gd.input1(123,"C7H16","2,4-dimethylpentane",atomName,atomN);
gd.input2(100.205,154.0,353.6,519.8,27.4,418.0,0.264,0.302,0.0);
double aCPC123[]={-7.046,0.6837,-3.734E-4,7.834E-8};aCPC=aCPC123;gd.input3(1,aCPC);
double aVPC123[]={-7.46358,1.43203,-3.42422,-2.20238};aVPC=aVPC123;gd.input4(1,aVPC);
gd.input5(-202100.0,3100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName124[]={"C","H"};atomName=atomName124;double atomN124[]={7.0,16.0};atomN=atomN124;
gd.input1(124,"C7H16","3,3-dimethylpentane",atomName,atomN);
gd.input2(100.205,138.7,359.2,536.4,29.5,414.0,0.273,0.267,0.0);
double aCPC124[]={-7.046,0.6837,-3.734E-4,7.834E-8};aCPC=aCPC124;gd.input3(1,aCPC);
double aVPC124[]={-7.49199,1.83146,-3.57292,-0.89448};aVPC=aVPC124;gd.input4(1,aVPC);
gd.input5(-201700.0,2640.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName125[]={"C","H"};atomName=atomName125;double atomN125[]={7.0,16.0};atomN=atomN125;
gd.input1(125,"C7H16","3-ethylpentane",atomName,atomN);
gd.input2(100.205,154.6,366.6,540.6,28.9,416.0,0.267,0.31,0.0);
double aCPC125[]={-7.046,0.6837,-3.734E-4,7.834E-8};aCPC=aCPC125;gd.input3(1,aCPC);
double aVPC125[]={-7.58305,1.58587,-3.56732,-2.42625};aVPC=aVPC125;gd.input4(1,aVPC);
gd.input5(-189800.0,11000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName126[]={"C","H"};atomName=atomName126;double atomN126[]={7.0,16.0};atomN=atomN126;
gd.input1(126,"C7H16","2,2,3-trimethylbutane",atomName,atomN);
gd.input2(100.205,248.3,354.0,531.2,29.5,398.0,0.266,0.25,0.0);
double aCPC126[]={-22.94,0.7519,-4.421E-4,1.005E-7};aCPC=aCPC126;gd.input3(1,aCPC);
double aVPC126[]={-7.22017,1.44914,-3.11808,-1.10598};aVPC=aVPC126;gd.input4(1,aVPC);
gd.input5(-204900.0,4270.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName127[]={"C","H","O"};atomName=atomName127;double atomN127[]={7.0,16.0,1.0};atomN=atomN127;
gd.input1(127,"C7H16O","1-heptanol",atomName,atomN);
gd.input2(116.204,239.2,449.8,633.0,30.4,435.0,0.251,0.56,1.7);
double aCPC127[]={49.07,0.6778,-3.447E-4,6.046E-8};aCPC=aCPC127;gd.input3(1,aCPC);
double aVPC127[]={8.6866,2626.42,-146.6,0.0};aVPC=aVPC127;gd.input4(3,aVPC);
gd.input5(-332000.0,-121000.0);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName128[]={"C","H","O"};atomName=atomName128;double atomN128[]={8.0,4.0,3.0};atomN=atomN128;
gd.input1(128,"C8H4O3","phthalicanhydride",atomName,atomN);
gd.input2(148.118,404.0,560.0,810.0,47.6,368.0,0.26,0.0,5.3);
double aCPC128[]={-4.455,0.654,-4.283E-4,1.009E-7};aCPC=aCPC128;gd.input3(1,aCPC);
double aVPC128[]={9.3782,4467.01,-83.15,0.0};aVPC=aVPC128;gd.input4(3,aVPC);
gd.input5(-371800.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName129[]={"C","H"};atomName=atomName129;double atomN129[]={8.0,8.0};atomN=atomN129;
gd.input1(129,"C8H8","styrene",atomName,atomN);
gd.input2(104.152,242.5,418.3,647.0,39.9,0.0,0.0,0.257,0.1);
double aCPC129[]={-28.25,0.6159,-4.023E-4,9.935E-8};aCPC=aCPC129;gd.input3(1,aCPC);
double aVPC129[]={-7.49199,1.83146,-3.57292,-0.89448};aVPC=aVPC129;gd.input4(1,aVPC);
gd.input5(145700.0,213900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName130[]={"C","H","O"};atomName=atomName130;double atomN130[]={8.0,8.0,1.0};atomN=atomN130;
gd.input1(130,"C8H8O","methylphenylketone",atomName,atomN);
gd.input2(120.151,292.8,474.9,714.0,40.6,376.0,0.257,0.42,3.0);
double aCPC130[]={-29.58,0.641,-4.071E-4,9.722E-8};aCPC=aCPC130;gd.input3(1,aCPC);
double aVPC130[]={-7.63896,1.24032,-3.60753,-1.55754};aVPC=aVPC130;gd.input4(1,aVPC);
gd.input5(-86920.0,1840.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName131[]={"C","H","O"};atomName=atomName131;double atomN131[]={8.0,8.0,2.0};atomN=atomN131;
gd.input1(131,"C8H8O2","methylbenzoate",atomName,atomN);
gd.input2(136.151,260.8,472.2,692.0,36.4,396.0,0.25,0.43,1.9);
double aCPC131[]={-21.21,0.5501,-1.799E-4,4.425E-8};aCPC=aCPC131;gd.input3(1,aCPC);
double aVPC131[]={9.607,3751.83,-81.15,0.0};aVPC=aVPC131;gd.input4(3,aVPC);
gd.input5(-254100.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName132[]={"C","H"};atomName=atomName132;double atomN132[]={8.0,10.0};atomN=atomN132;
gd.input1(132,"C8H10","o-xylene",atomName,atomN);
gd.input2(106.168,248.0,417.6,630.3,37.3,369.0,0.262,0.31,0.5);
double aCPC132[]={-15.85,0.5962,-3.443E-4,7.528E-8};aCPC=aCPC132;gd.input3(1,aCPC);
double aVPC132[]={-7.53357,1.40968,-3.10985,-2.85992};aVPC=aVPC132;gd.input4(1,aVPC);
gd.input5(19000.0,122200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName133[]={"C","H"};atomName=atomName133;double atomN133[]={8.0,10.0};atomN=atomN133;
gd.input1(133,"C8H10","m-xylene",atomName,atomN);
gd.input2(106.168,225.3,412.3,617.1,35.4,376.0,0.259,0.325,0.3);
double aCPC133[]={-29.17,0.6297,-3.747E-4,8.478E-8};aCPC=aCPC133;gd.input3(1,aCPC);
double aVPC133[]={-7.59222,1.39441,-3.22746,-2.40376};aVPC=aVPC133;gd.input4(1,aVPC);
gd.input5(17250.0,118900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName134[]={"C","H"};atomName=atomName134;double atomN134[]={8.0,10.0};atomN=atomN134;
gd.input1(134,"C8H10","p-xylene",atomName,atomN);
gd.input2(106.168,286.4,411.5,616.2,35.1,379.0,0.26,0.32,0.1);
double aCPC134[]={-25.09,0.6042,-3.374E-4,6.82};aCPC=aCPC134;gd.input3(1,aCPC);
double aVPC134[]={-7.63495,1.50724,-3.19678,-2.7871};aVPC=aVPC134;gd.input4(1,aVPC);
gd.input5(17960.0,121200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName135[]={"C","H","O"};atomName=atomName135;double atomN135[]={8.0,10.0,1.0};atomN=atomN135;
gd.input1(135,"C8H10O","ethylphenylether",atomName,atomN);
gd.input2(122.167,243.0,443.0,647.0,34.2,0.0,0.0,0.418,1.2);
double aCPC135[]={0.0,0.0,0.0,0.0};aCPC=aCPC135;gd.input3(1,aCPC);
double aVPC135[]={-8.50867,2.56997,-5.78999,0.10899};aVPC=aVPC135;gd.input4(1,aVPC);
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gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName136[]={"C","H","N"};atomName=atomName136;double atomN136[]={8.0,11.0,1.0};atomN=atomN136;
gd.input1(136,"C8H11N","N,N-dimethylaniline",atomName,atomN);
gd.input2(121.183,275.6,467.3,687.0,36.0,0.0,0.0,0.411,1.6);
double aCPC136[]={0.0,0.0,0.0,0.0};aCPC=aCPC136;gd.input3(1,aCPC);
double aVPC136[]={10.3445,4276.08,-52.8,0.0};aVPC=aVPC136;gd.input4(3,aVPC);
gd.input5(84150.0,231400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName137[]={"C","H"};atomName=atomName137;double atomN137[]={8.0,16.0};atomN=atomN137;
gd.input1(137,"C8H16","1,1-dimethylcyclohexane",atomName,atomN);
gd.input2(112.216,239.7,392.7,591.0,29.6,416.0,0.25,0.238,0.0);
double aCPC137[]={-72.11,0.8997,-5.02E-4,1.03E-7};aCPC=aCPC137;gd.input3(1,aCPC);
double aVPC137[]={-6.9281,1.01872,-3.04857,-1.70684};aVPC=aVPC137;gd.input4(1,aVPC);
gd.input5(-181100.0,35250.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName138[]={"C","H"};atomName=atomName138;double atomN138[]={8.0,16.0};atomN=atomN138;
gd.input1(138,"C8H16","1,2-dimethylcyclohexane-cis",atomName,atomN);
gd.input2(112.216,223.1,402.9,606.0,29.6,0.0,0.0,0.236,0.0);
double aCPC138[]={-68.37,0.8972,-5.137E-4,1.099E-7};aCPC=aCPC138;gd.input3(1,aCPC);
double aVPC138[]={-7.01944,1.3186,-3.96577,0.08142};aVPC=aVPC138;gd.input4(1,aVPC);
gd.input5(-172300.0,41240.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName139[]={"C","H"};atomName=atomName139;double atomN139[]={8.0,16.0};atomN=atomN139;
gd.input1(139,"C8H16","1,2-dimethylcyclohexane-trans",atomName,atomN);
gd.input2(112.216,185.0,396.6,596.0,29.6,0.0,0.0,0.242,0.0);
double aCPC139[]={-68.48,0.9123,-5.355E-4,1.181E-7};aCPC=aCPC139;gd.input3(1,aCPC);
double aVPC139[]={46.903,6162.66,-5.245,4785.0};aVPC=aVPC139;gd.input4(2,aVPC);
gd.input5(-180100.0,34500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName140[]={"C","H"};atomName=atomName140;double atomN140[]={8.0,16.0};atomN=atomN140;
gd.input1(140,"C8H16","1,3-dimethylcyclohexane-cis",atomName,atomN);
gd.input2(112.216,197.6,393.3,591.0,29.6,0.0,0.0,0.224,0.0);
double aCPC140[]={-65.16,0.8838,-4.932E-4,1.02E-7};aCPC=aCPC140;gd.input3(1,aCPC);
double aVPC140[]={9.1268,3081.95,-55.08,0.0};aVPC=aVPC140;gd.input4(3,aVPC);
gd.input5(-184900.0,29850.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName141[]={"C","H"};atomName=atomName141;double atomN141[]={8.0,16.0};atomN=atomN141;
gd.input1(141,"C8H16","1,3-dimethylcyclohexane-trans",atomName,atomN);
gd.input2(112.216,183.0,397.6,598.0,29.7,0.0,0.0,0.189,0.0);
double aCPC141[]={-64.15,0.8826,-5.016E-4,1.068E-7};aCPC=aCPC141;gd.input3(1,aCPC);
double aVPC141[]={49.477,6271.67,-5.615,4718.0};aVPC=aVPC141;gd.input4(2,aVPC);
gd.input5(-176700.0,36340.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName142[]={"C","H"};atomName=atomName142;double atomN142[]={8.0,16.0};atomN=atomN142;
gd.input1(142,"C8H16","1,4-dimethylcyclohexane-cis",atomName,atomN);
gd.input2(112.216,185.7,397.5,598.0,29.7,0.0,0.0,0.234,0.0);
double aCPC142[]={-64.15,0.8826,-5.016E-4,1.068E-7};aCPC=aCPC142;gd.input3(1,aCPC);
double aVPC142[]={46.951,6219.26,-5.233,4718.0};aVPC=aVPC142;gd.input4(2,aVPC);
gd.input5(-176800.0,37970.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName143[]={"C","H"};atomName=atomName143;double atomN143[]={8.0,16.0};atomN=atomN143;
gd.input1(143,"C8H16","1,4-dimethylcyclohexane-trans",atomName,atomN);
gd.input2(112.216,0.0,392.5,587.7,29.7,0.0,0.0,0.242,0.0);
double aCPC143[]={-70.36,0.9131,-5.309E-4,1.155E-7};aCPC=aCPC143;gd.input3(1,aCPC);
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double aVPC143[]={46.289,6071.72,-5.163,4650.0};aVPC=aVPC143;gd.input4(2,aVPC);
gd.input5(-184700.0,31740.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName144[]={"C","H"};atomName=atomName144;double atomN144[]={8.0,16.0};atomN=atomN144;
gd.input1(144,"C8H16","ethylcyclohexane",atomName,atomN);
gd.input2(112.216,161.8,404.9,609.0,30.0,450.0,0.27,0.243,0.0);
double aCPC144[]={-63.89,0.8893,-5.108E-4,1.103E-7};aCPC=aCPC144;gd.input3(1,aCPC);
double aVPC144[]={9.1923,3183.25,-58.15,0.0};aVPC=aVPC144;gd.input4(3,aVPC);
gd.input5(-171900.0,39270.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName145[]={"C","H"};atomName=atomName145;double atomN145[]={8.0,16.0};atomN=atomN145;
gd.input1(145,"C8H16","1,1,2-trimethylcyclopentane",atomName,atomN);
gd.input2(112.216,0.0,386.9,579.5,29.4,0.0,0.0,0.252,0.0);
double aCPC145[]={0.0,0.0,0.0,0.0};aCPC=aCPC145;gd.input3(1,aCPC);
double aVPC145[]={-7.01985,1.06194,-3.15886,-1.64858};aVPC=aVPC145;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName146[]={"C","H"};atomName=atomName146;double atomN146[]={8.0,16.0};atomN=atomN146;
gd.input1(146,"C8H16","1,1,3-trimethylcyclopentane",atomName,atomN);
gd.input2(112.216,0.0,378.0,569.5,28.3,0.0,0.0,0.211,0.0);
double aCPC146[]={0.0,0.0,0.0,0.0};aCPC=aCPC146;gd.input3(1,aCPC);
double aVPC146[]={-6.97215,1.62353,-4.90587,2.76293};aVPC=aVPC146;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName147[]={"C","H"};atomName=atomName147;double atomN147[]={8.0,16.0};atomN=atomN147;
gd.input1(147,"C8H16","1,2,4-trimethylcyclopentane-c,c,t",atomName,atomN);
gd.input2(112.216,0.0,391.0,579.0,29.0,0.0,0.0,0.277,0.0);
double aCPC147[]={0.0,0.0,0.0,0.0};aCPC=aCPC147;gd.input3(1,aCPC);
double aVPC147[]={9.1341,3073.95,-54.2,0.0};aVPC=aVPC147;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName148[]={"C","H"};atomName=atomName148;double atomN148[]={8.0,16.0};atomN=atomN148;
gd.input1(148,"C8H16","1,2,4-trimethylcyclopentane-c,t,c",atomName,atomN);
gd.input2(112.216,0.0,382.4,571.0,28.0,0.0,0.0,0.246,0.0);
double aCPC148[]={0.0,0.0,0.0,0.0};aCPC=aCPC148;gd.input3(1,aCPC);
double aVPC148[]={9.1554,3009.7,-53.23,0.0};aVPC=aVPC148;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName149[]={"C","H"};atomName=atomName149;double atomN149[]={8.0,16.0};atomN=atomN149;
gd.input1(149,"C8H16","1-methyl-1-ethylcyclopentane",atomName,atomN);
gd.input2(112.216,0.0,394.7,592.0,30.0,0.0,0.0,0.25,0.0);
double aCPC149[]={0.0,0.0,0.0,0.0};aCPC=aCPC149;gd.input3(1,aCPC);
double aVPC149[]={-7.09092,1.31715,-3.96332,0.30332};aVPC=aVPC149;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName150[]={"C","H"};atomName=atomName150;double atomN150[]={8.0,16.0};atomN=atomN150;
gd.input1(150,"C8H16","n-propylcyclopentane",atomName,atomN);
gd.input2(112.216,155.8,404.1,603.0,30.0,425.0,0.25,0.335,0.0);
double aCPC150[]={-55.97,0.8449,-4.924E-4,1.117E-7};aCPC=aCPC150;gd.input3(1,aCPC);
double aVPC150[]={-7.82031,2.88785,-6.85637,6.03561};aVPC=aVPC150;gd.input4(1,aVPC);
gd.input5(-148200.0,52630.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName151[]={"C","H"};atomName=atomName151;double atomN151[]={8.0,16.0};atomN=atomN151;
gd.input1(151,"C8H16","isopropylcyclopentane",atomName,atomN);
gd.input2(112.216,160.5,399.6,601.0,30.0,0.0,0.0,0.24,0.0);
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double aCPC151[]={0.0,0.0,0.0,0.0};aCPC=aCPC151;gd.input3(1,aCPC);
double aVPC151[]={-7.10096,1.54495,-4.66594,2.34067};aVPC=aVPC151;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName152[]={"C","H"};atomName=atomName152;double atomN152[]={8.0,16.0};atomN=atomN152;
gd.input1(152,"C8H16","cyclooctane",atomName,atomN);
gd.input2(112.216,287.6,422.0,647.2,35.6,410.0,0.271,0.236,0.0);
double aCPC152[]={0.0,0.0,0.0,0.0};aCPC=aCPC152;gd.input3(1,aCPC);
double aVPC152[]={9.1799,3310.62,-63.18,0.0};aVPC=aVPC152;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName153[]={"C","H"};atomName=atomName153;double atomN153[]={8.0,16.0};atomN=atomN153;
gd.input1(153,"C8H16","1-octene",atomName,atomN);
gd.input2(112.216,171.4,394.4,566.7,26.2,464.0,0.26,0.386,0.3);
double aCPC153[]={-4.099,0.7239,-4.036E-4,8.675E-8};aCPC=aCPC153;gd.input3(1,aCPC);
double aVPC153[]={57.867,6883.34,-6.765,5235.0};aVPC=aVPC153;gd.input4(2,aVPC);
gd.input5(-82980.0,104300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName154[]={"C","H"};atomName=atomName154;double atomN154[]={8.0,16.0};atomN=atomN154;
gd.input1(154,"C8H16","2-octene-trans",atomName,atomN);
gd.input2(112.216,185.4,398.1,580.0,27.7,0.0,0.0,0.35,0.0);
double aCPC154[]={-12.82,0.7532,-4.442E-4,1.05E-7};aCPC=aCPC154;gd.input3(1,aCPC);
double aVPC154[]={9.2352,3134.97,-58.0,0.0};aVPC=aVPC154;gd.input4(3,aVPC);
gd.input5(-94580.0,92740.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName155[]={"C","H","O"};atomName=atomName155;double atomN155[]={8.0,16.0,2.0};atomN=atomN155;
gd.input1(155,"C8H16O2","isobutylbutyrate",atomName,atomN);
gd.input2(144.214,0.0,430.1,603.0,24.5,0.0,0.0,0.0,0.0);
double aCPC155[]={0.0,0.0,0.0,0.0};aCPC=aCPC155;gd.input3(1,aCPC);
double aVPC155[]={-8.32597,1.4235,-4.25376,-3.09772};aVPC=aVPC155;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName156[]={"C","H","O"};atomName=atomName156;double atomN156[]={8.0,16.0,2.0};atomN=atomN156;
gd.input1(156,"C8H16O2","isobutylisobutyrate",atomName,atomN);
gd.input2(144.214,0.0,421.8,594.0,24.6,0.0,0.0,0.0,0.0);
double aCPC156[]={0.0,0.0,0.0,0.0};aCPC=aCPC156;gd.input3(1,aCPC);
double aVPC156[]={-8.18677,1.322,-3.94343,-3.68833};aVPC=aVPC156;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName157[]={"C","H","O"};atomName=atomName157;double atomN157[]={8.0,16.0,2.0};atomN=atomN157;
gd.input1(157,"C8H16O2","n-propylisovalerate",atomName,atomN);
gd.input2(144.214,0.0,429.1,609.0,0.0,0.0,0.0,0.0,0.0);
double aCPC157[]={0.0,0.0,0.0,0.0};aCPC=aCPC157;gd.input3(1,aCPC);
double aVPC157[]={0.0,0.0,0.0,0.0};aVPC=aVPC157;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName158[]={"C","H"};atomName=atomName158;double atomN158[]={8.0,18.0};atomN=atomN158;
gd.input1(158,"C8H18","2-methylheptane",atomName,atomN);
gd.input2(114.232,164.0,390.8,559.6,24.8,488.0,0.261,0.378,0.0);
double aCPC158[]={-89.7,1.242,-0.001176,4.618E-7};aCPC=aCPC158;gd.input3(1,aCPC);
double aVPC158[]={-7.80701,1.38191,-3.78286,-3.50395};aVPC=aVPC158;gd.input4(1,aVPC);
gd.input5(-215600.0,12770.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName159[]={"C","H"};atomName=atomName159;double atomN159[]={8.0,18.0};atomN=atomN159;
gd.input1(159,"C8H18","3-methylheptane",atomName,atomN);
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gd.input2(114.232,152.7,392.1,563.7,25.5,464.0,0.252,0.37,0.0);
double aCPC159[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC159;gd.input3(1,aCPC);
double aVPC159[]={-7.82876,1.50656,-3.86146,-3.52377};aVPC=aVPC159;gd.input4(1,aVPC);
gd.input5(-212800.0,13730.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName160[]={"C","H"};atomName=atomName160;double atomN160[]={8.0,18.0};atomN=atomN160;
gd.input1(160,"C8H18","4-methylheptane",atomName,atomN);
gd.input2(114.232,152.2,390.9,561.7,25.4,476.0,0.259,0.371,0.0);
double aCPC160[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC160;gd.input3(1,aCPC);
double aVPC160[]={-7.78757,1.40709,-3.76234,-3.50643};aVPC=aVPC160;gd.input4(1,aVPC);
gd.input5(-212200.0,16750.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName161[]={"C","H"};atomName=atomName161;double atomN161[]={8.0,18.0};atomN=atomN161;
gd.input1(161,"C8H18","2,2-dimethylhexane",atomName,atomN);
gd.input2(114.232,152.0,380.0,549.9,25.3,478.0,0.264,0.338,0.0);
double aCPC161[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC161;gd.input3(1,aCPC);
double aVPC161[]={-7.69898,1.56083,-3.75189,-3.01869};aVPC=aVPC161;gd.input4(1,aVPC);
gd.input5(-224900.0,10720.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName162[]={"C","H"};atomName=atomName162;double atomN162[]={8.0,18.0};atomN=atomN162;
gd.input1(162,"C8H18","2,3-dimethylhexane",atomName,atomN);
gd.input2(114.232,0.0,388.8,563.5,26.3,468.0,0.263,0.346,0.0);
double aCPC162[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC162;gd.input3(1,aCPC);
double aVPC162[]={-7.7518,1.58578,-3.80794,-2.58547};aVPC=aVPC162;gd.input4(1,aVPC);
gd.input5(-214100.0,17710.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName163[]={"C","H"};atomName=atomName163;double atomN163[]={8.0,18.0};atomN=atomN163;
gd.input1(163,"C8H18","2,4-dimethylhexane",atomName,atomN);
gd.input2(114.232,0.0,382.6,553.5,25.6,472.0,0.262,0.343,0.0);
double aCPC163[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC163;gd.input3(1,aCPC);
double aVPC163[]={-7.65152,1.41393,-3.62789,-3.06548};aVPC=aVPC163;gd.input4(1,aVPC);
gd.input5(-219600.0,11720.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName164[]={"C","H"};atomName=atomName164;double atomN164[]={8.0,18.0};atomN=atomN164;
gd.input1(164,"C8H18","2,5-dimethylhexane",atomName,atomN);
gd.input2(114.232,181.9,382.3,550.1,24.9,482.0,0.262,0.356,0.0);
double aCPC164[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC164;gd.input3(1,aCPC);
double aVPC164[]={-7.76508,1.51236,-3.78809,-3.07843};aVPC=aVPC164;gd.input4(1,aVPC);
gd.input5(-222800.0,10470.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName165[]={"C","H"};atomName=atomName165;double atomN165[]={8.0,18.0};atomN=atomN165;
gd.input1(165,"C8H18","3,3-dimethylhexane",atomName,atomN);
gd.input2(114.232,147.0,385.1,562.0,26.5,443.0,0.251,0.32,0.0);
double aCPC165[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC165;gd.input3(1,aCPC);
double aVPC165[]={-7.59847,1.50336,-3.49912,-2.38236};aVPC=aVPC165;gd.input4(1,aVPC);
gd.input5(-220300.0,13270.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName166[]={"C","H"};atomName=atomName166;double atomN166[]={8.0,18.0};atomN=atomN166;
gd.input1(166,"C8H18","3,4-dimethylhexane",atomName,atomN);
gd.input2(114.232,0.0,390.9,568.9,26.9,466.0,0.265,0.338,0.0);
double aCPC166[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC166;gd.input3(1,aCPC);
double aVPC166[]={-7.72976,1.61174,-3.75756,-2.62874};aVPC=aVPC166;gd.input4(1,aVPC);
gd.input5(-213100.0,17330.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName167[]={"C","H"};atomName=atomName167;double atomN167[]={8.0,18.0};atomN=atomN167;
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gd.input1(167,"C8H18","3-ethylhexane",atomName,atomN);
gd.input2(114.232,0.0,391.7,565.5,26.1,455.0,0.252,0.361,0.0);
double aCPC167[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC167;gd.input3(1,aCPC);
double aVPC167[]={-7.75246,1.42908,-3.68445,-3.46671};aVPC=aVPC167;gd.input4(1,aVPC);
gd.input5(-211000.0,16940.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName168[]={"C","H"};atomName=atomName168;double atomN168[]={8.0,18.0};atomN=atomN168;
gd.input1(168,"C8H18","2,2,3-trimethylpentane",atomName,atomN);
gd.input2(114.232,160.9,383.0,563.5,27.3,436.0,0.254,0.297,0.0);
double aCPC168[]={-9.215,0.7859,-4.4E-4,9.697E-8};aCPC=aCPC168;gd.input3(1,aCPC);
double aVPC168[]={-7.48839,1.52208,-3.44481,-2.12538};aVPC=aVPC168;gd.input4(1,aVPC);
gd.input5(-220300.0,17120.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName169[]={"C","H"};atomName=atomName169;double atomN169[]={8.0,18.0};atomN=atomN169;
gd.input1(169,"C8H18","2,2,4-trimethylpentane",atomName,atomN);
gd.input2(114.232,165.8,372.4,544.0,25.7,468.0,0.266,0.303,0.0);
double aCPC169[]={-7.461,-0.7779,-4.287E-4,9.173E-8};aCPC=aCPC169;gd.input3(1,aCPC);
double aVPC169[]={-7.3889,1.25294,-3.16606,-2.22001};aVPC=aVPC169;gd.input4(1,aVPC);
gd.input5(-224300.0,13690.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName170[]={"C","H"};atomName=atomName170;double atomN170[]={8.0,18.0};atomN=atomN170;
gd.input1(170,"C8H18","2,2,3,3-tetramethylbutane",atomName,atomN);
gd.input2(114.232,374.0,379.6,567.8,28.7,461.0,0.28,0.251,0.0);
double aCPC170[]={0.0,0.0,0.0,0.0};aCPC=aCPC170;gd.input3(1,aCPC);
double aVPC170[]={11.4937,3856.39,-42.42,0.0};aVPC=aVPC170;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName171[]={"C","H","O"};atomName=atomName171;double atomN171[]={8.0,18.0,1.0};atomN=atomN171;
gd.input1(171,"C8H18O","1-octanol",atomName,atomN);
gd.input2(130.231,257.7,468.3,652.5,28.6,490.0,0.258,0.587,2.0);
double aCPC171[]={6.171,0.7607,-3.797E-4,6.263E-8};aCPC=aCPC171;gd.input3(1,aCPC);
double aVPC171[]={-9.71763,4.22514,-12.9222,-3.59254};aVPC=aVPC171;gd.input4(1,aVPC);
gd.input5(-360100.0,-120200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName172[]={"C","H","O"};atomName=atomName172;double atomN172[]={8.0,18.0,1.0};atomN=atomN172;
gd.input1(172,"C8H18O","2-octanol",atomName,atomN);
gd.input2(130.231,241.2,452.0,637.0,28.1,0.0,0.0,0.0,1.6);
double aCPC172[]={25.88,0.7641,-4.224E-4,9.064E-8};aCPC=aCPC172;gd.input3(1,aCPC);
double aVPC172[]={8.0906,2441.66,-150.7,0.0};aVPC=aVPC172;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName173[]={"C","H","O"};atomName=atomName173;double atomN173[]={8.0,18.0,1.0};atomN=atomN173;
gd.input1(173,"C8H18O","4-methyl-3-heptanol",atomName,atomN);
gd.input2(130.231,0.0,443.0,623.5,28.0,0.0,0.0,0.0,0.0);
double aCPC173[]={0.0,0.0,0.0,0.0};aCPC=aCPC173;gd.input3(1,aCPC);
double aVPC173[]={0.0,0.0,0.0,0.0};aVPC=aVPC173;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName174[]={"C","H","O"};atomName=atomName174;double atomN174[]={8.0,18.0,1.0};atomN=atomN174;
gd.input1(174,"C8H18O","5-methyl-3-heptanol",atomName,atomN);
gd.input2(130.231,0.0,445.0,621.2,0.0,0.0,0.0,0.0,0.0);
double aCPC174[]={0.0,0.0,0.0,0.0};aCPC=aCPC174;gd.input3(1,aCPC);
double aVPC174[]={0.0,0.0,0.0,0.0};aVPC=aVPC174;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
```

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String atomName175[]={"C","H","O"};atomName=atomName175;double atomN175[]={8.0,18.0,1.0};atomN=atomN175;
gd.input1(175,"C8H18O","2-ethyl-1-hexanol",atomName,atomN);
gd.input2(130.231,203.2,457.8,640.2,0.0,0.0,0.0,0.0,1.8);
double aCPC175[]={-14.99,0.8645,-5.28E-4,1.285E-7};aCPC=aCPC175;gd.input3(1,aCPC);
double aVPC175[]={8.7412,2772.46,-140.0,0.0};aVPC=aVPC175;gd.input4(3,aVPC);
gd.input5(-365500.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName176[]={"C","H","O"};atomName=atomName176;double atomN176[]={8.0,18.0,1.0};atomN=atomN176;
gd.input1(176,"C8H18O","dibutylether",atomName,atomN);
gd.input2(130.231,175.0,413.4,580.0,25.3,0.0,0.0,0.502,1.2);
double aCPC176[]={6.054,0.7729,-4.085E-4,8.085E-8};aCPC=aCPC176;gd.input3(1,aCPC);
double aVPC176[]={-9.0497,2.78734,-5.11686,-3.97104};aVPC=aVPC176;gd.input4(1,aVPC);
gd.input5(-334100.0,-88590.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName177[]={"C","H","O"};atomName=atomName177;double atomN177[]={8.0,18.0,1.0};atomN=atomN177;
gd.input1(177,"C8H18O","di-tert-butylether",atomName,atomN);
gd.input2(130.231,0.0,382.2,550.0,24.2,0.0,0.0,0.0,0.0);
double aCPC177[]={0.0,0.0,0.0,0.0};aCPC=aCPC177;gd.input3(1,aCPC);
double aVPC177[]={-7.47062,1.33672,-4.00322,-1.89122};aVPC=aVPC177;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName178[]={"C","H","N"};atomName=atomName178;double atomN178[]={8.0,19.0,1.0};atomN=atomN178;
gd.input1(178,"C8H19N","dibutylamin",atomName,atomN);
gd.input2(129.247,211.0,432.8,607.5,26.4,0.0,0.0,0.58,1.1);
double aCPC178[]={9.764,0.8081,-4.329E-4,9.249E-8};aCPC=aCPC178;gd.input3(1,aCPC);
double aVPC178[]={-9.14853,2.93179,-6.02092,0.93342};aVPC=aVPC178;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName179[]={"C","H","N"};atomName=atomName179;double atomN179[]={8.0,19.0,1.0};atomN=atomN179;
gd.input1(179,"C8H19N","diisobutylamine",atomName,atomN);
gd.input2(129.247,203.0,412.8,584.4,27.2,0.0,0.0,0.548,0.0);
double aCPC179[]={0.0,0.0,0.0,0.0};aCPC=aCPC179;gd.input3(1,aCPC);
double aVPC179[]={-8.95962,2.85335,-5.81427,0.65701};aVPC=aVPC179;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName180[]={"C","H","N"};atomName=atomName180;double atomN180[]={9.0,7.0,1.0};atomN=atomN180;
gd.input1(180,"C9H7N","quinoline",atomName,atomN);
gd.input2(129.162,258.0,510.8,782.0,45.0,402.0,0.278,0.315,0.0);
double aCPC180[]={0.0,0.0,0.0,0.0};aCPC=aCPC180;gd.input3(1,aCPC);
double aVPC180[]={9.0779,3842.4,-86.94,0.0};aVPC=aVPC180;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName181[]={"C","H","N"};atomName=atomName181;double atomN181[]={9.0,7.0,1.0};atomN=atomN181;
gd.input1(181,"C9H7N","isoquinoline",atomName,atomN);
gd.input2(129.162,300.0,516.4,803.0,47.0,402.0,0.283,0.0,0.0);
double aCPC181[]={0.0,0.0,0.0,0.0};aCPC=aCPC181;gd.input3(1,aCPC);
double aVPC181[]={9.2957,3968.37,-88.94,0.0};aVPC=aVPC181;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName182[]={"C","H"};atomName=atomName182;double atomN182[]={9.0,10.0};atomN=atomN182;
gd.input1(182,"C9H10","indane",atomName,atomN);
gd.input2(118.179,0.0,451.1,684.9,39.5,0.0,0.0,0.308,0.0);
double aCPC182[]={0.0,0.0,0.0,0.0};aCPC=aCPC182;gd.input3(1,aCPC);
double aVPC182[]={0.0,0.0,0.0,0.0};aVPC=aVPC182;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName183[]={"C","H"};atomName=atomName183;double atomN183[]={9.0,10.0};atomN=atomN183;
gd.input1(183,"C9H10","alpha-methylstyrene",atomName,atomN);
gd.input2(118.179,0.0,438.5,654.0,34.0,0.0,0.0,0.0,0.0);
double aCPC183[]={-24.33,0.6933,-4.53E-4,1.181E-7};aCPC=aCPC183;gd.input3(1,aCPC);
double aVPC183[]={9.7106,3644.3,-67.15,0.0};aVPC=aVPC183;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName184[]={"C","H","O"};atomName=atomName184;double atomN184[]={9.0,10.0,2.0};atomN=atomN184;
gd.input1(184,"C9H10O2","ethylbenzoate",atomName,atomN);
gd.input2(150.178,238.3,485.9,668.7,23.2,0.0,0.0,0.48,0.0);
double aCPC184[]={20.67,0.6887,-3.608E-4,5.062E-8};aCPC=aCPC184;gd.input3(1,aCPC);
double aVPC184[]={-9.32936,2.89807,-6.54578,5.56703};aVPC=aVPC184;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName185[]={"C","H"};atomName=atomName185;double atomN185[]={9.0,12.0};atomN=atomN185;
gd.input1(185,"C9H12","n-propylbenzene",atomName,atomN);
gd.input2(120.195,173.7,432.4,638.2,32.0,440.0,0.265,0.344,0.0);
double aCPC185[]={-31.29,0.7468,-4.601E-4,1.081E-7};aCPC=aCPC185;gd.input3(1,aCPC);
double aVPC185[]={-7.92198,1.97403,-4.27504,-1.28568};aVPC=aVPC185;gd.input4(1,aVPC);
gd.input5(7830.0,137300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName186[]={"C","H"};atomName=atomName186;double atomN186[]={9.0,12.0};atomN=atomN186;
gd.input1(186,"C9H12","isopropylbenzene",atomName,atomN);
gd.input2(120.195,177.1,425.6,631.1,32.1,0.0,0.0,0.326,0.0);
double aCPC186[]={-39.36,0.7842,-5.078E-4,1.291E-7};aCPC=aCPC186;gd.input3(1,aCPC);
double aVPC186[]={-7.46042,1.14486,-3.19082,-3.62628};aVPC=aVPC186;gd.input4(1,aVPC);
gd.input5(3940.0,137100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName187[]={"C","H"};atomName=atomName187;double atomN187[]={9.0,12.0};atomN=atomN187;
gd.input1(187,"C9H12","1-methyl-3-ethylbenzene",atomName,atomN);
gd.input2(120.195,177.6,434.5,637.0,28.4,490.0,0.26,0.36,0.0);
double aCPC187[]={-29.0,0.7293,-4.363E-4,9.998E-8};aCPC=aCPC187;gd.input3(1,aCPC);
double aVPC187[]={-7.86301,2.47961,-6.98644,6.35609};aVPC=aVPC187;gd.input4(1,aVPC);
gd.input5(-1930.0,126500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName188[]={"C","H"};atomName=atomName188;double atomN188[]={9.0,12.0};atomN=atomN188;
gd.input1(188,"C9H12","1-methyl-4-ethylbenzene",atomName,atomN);
gd.input2(120.195,210.8,435.2,640.0,29.4,470.0,0.26,0.322,0.0);
double aCPC188[]={-27.31,0.7176,-4.224E-4,9.542E-8};aCPC=aCPC188;gd.input3(1,aCPC);
double aVPC188[]={-7.68892,1.92198,-5.66712,2.28086};aVPC=aVPC188;gd.input4(1,aVPC);
gd.input5(-2050.0,126800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName189[]={"C","H"};atomName=atomName189;double atomN189[]={9.0,12.0};atomN=atomN189;
gd.input1(189,"C9H12","1,2,3-trimethylbenzene",atomName,atomN);
gd.input2(120.195,247.7,449.3,664.5,34.5,0.0,0.0,0.366,0.0);
double aCPC189[]={-6.942,0.6335,-3.326E-4,6.611E-8};aCPC=aCPC189;gd.input3(1,aCPC);
double aVPC189[]={-8.44191,2.92198,-5.66712,2.28086};aVPC=aVPC189;gd.input4(1,aVPC);
gd.input5(-9590.0,124600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName190[]={"C","H"};atomName=atomName190;double atomN190[]={9.0,12.0};atomN=atomN190;
gd.input1(190,"C9H12","1,2,4-trimethylbenzene",atomName,atomN);
gd.input2(120.195,227.0,442.5,649.2,32.3,0.0,0.0,0.376,0.0);
double aCPC190[]={-4.668,0.6238,-3.263E-4,6.376E-8};aCPC=aCPC190;gd.input3(1,aCPC);
double aVPC190[]={-8.50002,2.98227,-6.02665,3.51307};aVPC=aVPC190;gd.input4(1,aVPC);
gd.input5(-13940.0,117000.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName191[]={"C","H"};atomName=atomName191;double atomN191[]={9.0,12.0};atomN=atomN191;
gd.input1(191,"C9H12","1,3,5-trimethylbenzene",atomName,atomN);
gd.input2(120.195,228.4,437.9,637.3,31.3,0.0,0.0,0.399,0.1);
double aCPC191[]={-19.59,0.6724,-3.629E-4,7.7E-8};aCPC=aCPC191;gd.input3(1,aCPC);
double aVPC191[]={-8.3715,2.41166,-5.30321,2.67635};aVPC=aVPC191;gd.input4(1,aVPC);
gd.input5(-16080.0,118000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName192[]={"C","H","N"};atomName=atomName192;double atomN192[]={9.0,13.0,1.0};atomN=atomN192;
gd.input1(192,"C9H13N","N,N-dimethyl-o-toluidine",atomName,atomN);
gd.input2(135.21,212.0,467.3,668.0,31.2,0.0,0.0,0.484,0.9);
double aCPC192[]={0.0,0.0,0.0,0.0};aCPC=aCPC192;gd.input3(1,aCPC);
double aVPC192[]={0.0,0.0,0.0,0.0};aVPC=aVPC192;gd.input4(2,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName193[]={"C","H"};atomName=atomName193;double atomN193[]={9.0,18.0};atomN=atomN193;
gd.input1(193,"C9H18","n-propylcyclohexane",atomName,atomN);
gd.input2(126.243,178.7,429.9,639.0,28.0,0.0,0.0,0.258,0.0);
double aCPC193[]={-62.52,0.9889,-5.795E-4,1.291E-7};aCPC=aCPC193;gd.input3(1,aCPC);
double aVPC193[]={-7.37782,2.13149,-6.45979,5.82529};aVPC=aVPC193;gd.input4(1,aVPC);
gd.input5(-193400.0,47350.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName194[]={"C","H"};atomName=atomName194;double atomN194[]={9.0,18.0};atomN=atomN194;
gd.input1(194,"C9H18","isopropylcyclohexane",atomName,atomN);
gd.input2(126.0,243.0,183.4,427.7,640.0,28.3,0.0,0.0,0.237);
double aCPC194[]={0.0,0.0,0.0,0.0};aCPC=aCPC194;gd.input3(1,aCPC);
double aVPC194[]={-7.24565,2.09643,-6.35158,5.5038};aVPC=aVPC194;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName195[]={"C","H"};atomName=atomName195;double atomN195[]={9.0,18.0};atomN=atomN195;
gd.input1(195,"C9H18","1,trans-3,5-trimethylcyclohexane",atomName,atomN);
gd.input2(126.243,0.0,413.7,602.2,28.0,0.0,0.0,0.0,0.0);
double aCPC195[]={0.0,0.0,0.0,0.0};aCPC=aCPC195;gd.input3(1,aCPC);
double aVPC195[]={0.0,0.0,0.0,0.0};aVPC=aVPC195;gd.input4(2,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName196[]={"C","H"};atomName=atomName196;double atomN196[]={9.0,18.0};atomN=atomN196;
gd.input1(196,"C9H18","1-nonene",atomName,atomN);
gd.input2(126.243,191.8,420.0,592.0,23.4,580.0,0.28,0.43,0.0);
double aCPC196[]={-3.718,0.8122,-4.509E-4,9.705E-8};aCPC=aCPC196;gd.input3(1,aCPC);
double aVPC196[]={-8.30824,2.03357,-5.42753,0.95331};aVPC=aVPC196;gd.input4(1,aVPC);
gd.input5(-103600.0,112800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName197[]={"C","H","O"};atomName=atomName197;double atomN197[]={9.0,18.0,1.0};atomN=atomN197;
gd.input1(197,"C9H18O","dibutylketone",atomName,atomN);
gd.input2(142.242,267.3,461.6,640.0,0.0,0.0,0.0,0.0,2.7);
double aCPC197[]={0.0,0.0,0.0,0.0};aCPC=aCPC197;gd.input3(1,aCPC);
double aVPC197[]={0.0,0.0,0.0,0.0};aVPC=aVPC197;gd.input4(2,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName198[]={"C","H"};atomName=atomName198;double atomN198[]={9.0,20.0};atomN=atomN198;
gd.input1(198,"C9H20","2-methyloctane",atomName,atomN);
gd.input2(128.242,192.8,416.4,587.0,23.1,0.0,0.0,0.423,0.0);
double aCPC198[]={-10.11,0.8805,-4.936E-4,1.083E-7};aCPC=aCPC198;gd.input3(1,aCPC);
double aVPC198[]={9.3089,3246.64,-67.2,0.0};aVPC=aVPC198;gd.input4(3,aVPC);
gd.input5(-229200.0,24830.0);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName199[]={"C","H"};atomName=atomName199;double atomN199[]={9.0,20.0};atomN=atomN199;
gd.input1(199,"C9H20","2,2-dimethylheptane",atomName,atomN);
gd.input2(128.242,160.0,405.9,576.8,23.5,0.0,0.0,0.39,0.0);
double aCPC199[]={-20.89,0.9668,-6.12E-4,1.57E-7};aCPC=aCPC199;gd.input3(1,aCPC);
double aVPC199[]={9.1717,3120.0,-65.2,0.0};aVPC=aVPC199;gd.input4(3,aVPC);
gd.input5(-247000.0,16750.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName200[]={"C","H"};atomName=atomName200;double atomN200[]={9.0,20.0};atomN=atomN200;
gd.input1(200,"C9H20","2,2,3-trimethylhexane",atomName,atomN);
gd.input2(128.259,0.0,406.8,588.0,24.9,0.0,0.0,0.332,0.0);
double aCPC200[]={-45.63,1.055,-7.172E-4,1.987E-7};aCPC=aCPC200;gd.input3(1,aCPC);
double aVPC200[]={9.1815,3164.17,-61.66,0.0};aVPC=aVPC200;gd.input4(3,aVPC);
gd.input5(-241400.0,24530.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName201[]={"C","H"};atomName=atomName201;double atomN201[]={9.0,20.0};atomN=atomN201;
gd.input1(201,"C9H20","2,2,4-trimethylhexane",atomName,atomN);
gd.input2(128.259,153.0,399.7,573.7,23.7,0.0,0.0,0.321,0.0);
double aCPC201[]={-60.31,1.104,-7.712E-4,2.188E-7};aCPC=aCPC201;gd.input3(1,aCPC);
double aVPC201[]={9.1437,3084.08,-61.94,0.0};aVPC=aVPC201;gd.input4(3,aVPC);
gd.input5(-243400.0,22520.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName202[]={"C","H"};atomName=atomName202;double atomN202[]={9.0,20.0};atomN=atomN202;
gd.input1(202,"C9H20","2,2,5-trimethylhexane",atomName,atomN);
gd.input2(128.259,167.4,397.2,568.0,23.3,519.0,0.26,0.357,0.0);
double aCPC202[]={-54.11,1.095,-7.746E-4,2.255E-7};aCPC=aCPC202;gd.input3(1,aCPC);
double aVPC202[]={-7.80573,1.68023,-4.50859,-0.78808};aVPC=aVPC202;gd.input4(1,aVPC);
gd.input5(-252400.0,13440.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName203[]={"C","H"};atomName=atomName203;double atomN203[]={9.0,20.0};atomN=atomN203;
gd.input1(203,"C9H20","3,3-diethylpentane",atomName,atomN);
gd.input2(128.259,240.1,419.3,610.0,26.7,0.0,0.0,0.338,0.0);
double aCPC203[]={-67.27,1.126,-7.988E-4,2.306E-7};aCPC=aCPC203;gd.input3(1,aCPC);
double aVPC203[]={-7.98732,2.15446,-4.25035,-0.09787};aVPC=aVPC203;gd.input4(1,aVPC);
gd.input5(-232100.0,35090.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName204[]={"C","H"};atomName=atomName204;double atomN204[]={9.0,20.0};atomN=atomN204;
gd.input1(204,"C9H20","2,2,3,3-tetramethylpentane",atomName,atomN);
gd.input2(128.259,263.0,413.4,607.7,27.4,0.0,0.0,0.303,0.0);
double aCPC204[]={-54.58,1.089,-7.57E-4,2.142E-7};aCPC=aCPC204;gd.input3(1,aCPC);
double aVPC204[]={-7.40615,1.23976,-2.94462,-3.35833};aVPC=aVPC204;gd.input4(1,aVPC);
gd.input5(-237400.0,34330.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName205[]={"C","H"};atomName=atomName205;double atomN205[]={9.0,20.0};atomN=atomN205;
gd.input1(205,"C9H20","2,2,3,4-tetramethylpentane",atomName,atomN);
gd.input2(128.259,152.0,406.1,592.7,26.0,0.0,0.0,0.313,0.0);
double aCPC205[]={-54.58,1.089,-7.57E-4,2.142E-7};aCPC=aCPC205;gd.input3(1,aCPC);
double aVPC205[]={-7.60624,1.62208,-3.71777,-1.50403};aVPC=aVPC205;gd.input4(1,aVPC);
gd.input5(-237100.0,32660.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName206[]={"C","H"};atomName=atomName206;double atomN206[]={9.0,20.0};atomN=atomN206;
gd.input1(206,"C9H20","2,2,4,4-tetramethylpentane",atomName,atomN);
gd.input2(128.259,206.0,395.4,574.7,24.9,0.0,0.0,0.312,0.0);
double aCPC206[]={-67.4,1.168,-8.612E-4,2.574E-7};aCPC=aCPC206;gd.input3(1,aCPC);
double aVPC206[]={-7.7157,1.89775,-4.0894,-0.7541};aVPC=aVPC206;gd.input4(1,aVPC);
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gd.input5(-242100.0,34040.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName207[]={"C","H"};atomName=atomName207;double atomN207[]={9.0,20.0};atomN=atomN207;
gd.input1(207,"C9H20","2,3,3,4-tetramethylpentane",atomName,atomN);
gd.input2(128.259,171.1,414.7,607.7,27.2,0.0,0.0,0.313,0.0);
double aCPC207[]={-54.92,1.091,-7.603E-4,2.158E-7};aCPC=aCPC207;gd.input3(1,aCPC);
double aVPC207[]={-7.65,1.71897,-3.82026,-0.95911};aVPC=aVPC207;gd.input4(1,aVPC);
gd.input5(-236400.0,34120.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName208[]={"C","H","O"};atomName=atomName208;double atomN208[]={9.0,20.0,1.0};atomN=atomN208;
gd.input1(208,"C9H20O","1-nonanol",atomName,atomN);
gd.input2(144.258,268.0,486.7,671.0,0.0,546.0,0.0,0.0,1.7);
double aCPC208[]={1.28,0.8817,-4.791E-4,9.801E-8};aCPC=aCPC208;gd.input3(1,aCPC);
double aVPC208[]={8.7513,2939.54,-150.1,0.0};aVPC=aVPC208;gd.input4(3,aVPC);
gd.input5(-387200.0,-118300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName209[]={"C","F"};atomName=atomName209;double atomN209[]={10.0,8.0};atomN=atomN209;
gd.input1(209,"C10F8","perfluoronapthalene",atomName,atomN);
gd.input2(272.094,0.0,482.0,673.1,0.0,0.0,0.0,0.0,0.0);
double aCPC209[]={0.0,0.0,0.0,0.0};aCPC=aCPC209;gd.input3(1,aCPC);
double aVPC209[]={0.0,0.0,0.0,0.0};aVPC=aVPC209;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName210[]={"C","F"};atomName=atomName210;double atomN210[]={10.0,18.0};atomN=atomN210;
gd.input1(210,"C10F18","perfluorodecalin",atomName,atomN);
gd.input2(462.074,0.0,415.0,566.0,15.2,0.0,0.0,0.392,0.0);
double aCPC210[]={0.0,0.0,0.0,0.0};aCPC=aCPC210;gd.input3(1,aCPC);
double aVPC210[]={0.0,0.0,0.0,0.0};aVPC=aVPC210;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName211[]={"C","H"};atomName=atomName211;double atomN211[]={10.0,12.0};atomN=atomN211;
gd.input1(211,"C10H12","1,2,3,4-tetrahydronaphthalene",atomName,atomN);
gd.input2(132.206,242.0,480.7,719.0,35.1,0.0,0.0,0.303,0.0);
double aCPC211[]={0.0,0.0,0.0,0.0};aCPC=aCPC211;gd.input3(1,aCPC);
double aVPC211[]={9.5883,4009.49,-64.89,0.0};aVPC=aVPC211;gd.input4(3,aVPC);
gd.input5(2760.0,167100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName212[]={"C","H"};atomName=atomName212;double atomN212[]={10.0,14.0};atomN=atomN212;
gd.input1(212,"C10H14","n-butylbenzene",atomName,atomN);
gd.input2(134.22,185.2,456.5,660.5,28.9,497.0,0.261,0.393,0.4);
double aCPC212[]={-22.99,0.7934,-4.396E-4,8.57E-8};aCPC=aCPC212;gd.input3(1,aCPC);
double aVPC212[]={-8.39978,2.61916,-5.80532,2.11591};aVPC=aVPC212;gd.input4(1,aVPC);
gd.input5(-13820.0,144800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName213[]={"C","H"};atomName=atomName213;double atomN213[]={10.0,14.0};atomN=atomN213;
gd.input1(213,"C10H14","isobutylbenzene",atomName,atomN);
gd.input2(134.222,221.7,445.9,650.0,31.4,480.0,0.28,0.38,0.3);
double aCPC213[]={0.0,0.0,0.0,0.0};aCPC=aCPC213;gd.input3(1,aCPC);
double aVPC213[]={-8.13153,1.58186,-2.37146,-7.46781};aVPC=aVPC213;gd.input4(1,aVPC);
gd.input5(-21560.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName214[]={"C","H"};atomName=atomName214;double atomN214[]={10.0,14.0};atomN=atomN214;
gd.input1(214,"C10H14","sec-butylbenzene",atomName,atomN);
gd.input2(134.222,197.7,446.5,664.0,29.4,0.0,0.0,0.274,0.4);
double aCPC214[]={-65.15,0.9893,-7.214E-4,2.152E-7};aCPC=aCPC214;gd.input3(1,aCPC);
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double aVPC214[]={-7.49482,2.2344,-6.77346,6.31118};aVPC=aVPC214;gd.input4(1,aVPC);
gd.input5(-17460.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName215[]={"C","H"};atomName=atomName215;double atomN215[]={10.0,14.0};atomN=atomN215;
gd.input1(215,"C10H14","tert-butylbenzene",atomName,atomN);
gd.input2(134.222,215.3,442.3,660.0,29.6,0.0,0.0,0.265,0.5);
double aCPC215[]={-86.0,1.102,-8.746E-4,2.827E-7};aCPC=aCPC215;gd.input3(1,aCPC);
double aVPC215[]={-7.45802,2.33227,-7.07129,6.72178};aVPC=aVPC215;gd.input4(1,aVPC);
gd.input5(-22690.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName216[]={"C","H"};atomName=atomName216;double atomN216[]={10.0,14.0};atomN=atomN216;
gd.input1(216,"C10H14","1-methyl-2-isopropylbenzene",atomName,atomN);
gd.input2(134.222,0.0,451.5,670.0,28.9,0.0,0.0,0.277,0.0);
double aCPC216[]={0.0,0.0,0.0,0.0};aCPC=aCPC216;gd.input3(1,aCPC);
double aVPC216[]={9.3607,3564.52,-70.0,0.0};aVPC=aVPC216;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName217[]={"C","H"};atomName=atomName217;double atomN217[]={10.0,14.0};atomN=atomN217;
gd.input1(217,"C10H14","1-methyl-3-isopropylbenzene",atomName,atomN);
gd.input2(134.222,0.0,448.3,666.0,29.3,0.0,0.0,0.279,0.0);
double aCPC217[]={-48.76,0.9064,-6.054E-4,1.627E-7};aCPC=aCPC217;gd.input3(1,aCPC);
double aVPC217[]={61.106,8033.58,-7.076,6293.0};aVPC=aVPC217;gd.input4(2,aVPC);
gd.input5(-29310.0,0.0);
gi.addElement(gd);}
  public void data3()
 {Gas_Data gd=new Gas_Data();
String atomName218[]={"C","H"};atomName=atomName218;double atomN218[]={10.0,14.0};atomN=atomN218;
gd.input1(218,"C10H14","1-methyl-4-isopropylbenzene",atomName,atomN);
gd.input2(134.222,200.0,450.3,651.0,27.3,0.0,0.0,0.273,0.0);
double aCPC218[]={0.0,0.0,0.0,0.0};aCPC=aCPC218;gd.input3(1,aCPC);
double aVPC218[]={56.605,7800.97,-6.432,6308.0};aVPC=aVPC218;gd.input4(2,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName219[]={"C","H"};atomName=atomName219;double atomN219[]={10.0,14.0};atomN=atomN219;
gd.input1(219,"C10H14","1,4-diethylbenzene",atomName,atomN);
gd.input2(134.222,231.0,456.9,657.9,28.0,0.0,0.0,0.404,0.1);
double aCPC219[]={-37.42,0.8671,-5.56E-4,1.411E-7};aCPC=aCPC219;gd.input3(1,aCPC);
double aVPC219[]={-8.11413,1.77697,-4.4369,-1.47477};aVPC=aVPC219;gd.input4(1,aVPC);
gd.input5(-22270.0,138000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName220[]={"C","H"};atomName=atomName220;double atomN220[]={10.0,14.0};atomN=atomN220;
gd.input1(220,"C10H14","1,2,3,5-tetramethylbenzene",atomName,atomN);
gd.input2(134.222,249.0,471.2,679.0,0.0,0.0,0.0,0.0,0.0);
double aCPC220[]={3.923,0.7131,-3.711E-4,6.84E-8};aCPC=aCPC220;gd.input3(1,aCPC);
double aVPC220[]={9.675,3854.53,-72.26,0.0};aVPC=aVPC220;gd.input4(3,aVPC);
gd.input5(-44840.0,118800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName221[]={"C","H"};atomName=atomName221;double atomN221[]={10.0,14.0};atomN=atomN221;
gd.input1(221,"C10H14","1,2,4,5-tetramethylbenzene",atomName,atomN);
gd.input2(134.212,352.0,470.0,675.0,29.4,0.0,0.0,0.435,0.0);
double aCPC221[]={16.25,0.6519,-2.879E-4,3.257E-8};aCPC=aCPC221;gd.input3(1,aCPC);
double aVPC221[]={57.519,8300.92,-6.478,6600.0};aVPC=aVPC221;gd.input4(2,aVPC);
gd.input5(-45300.0,119500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName222[]={"C","H","O"};atomName=atomName222;double atomN222[]={10.0,14.0,1.0};atomN=atomN222;
gd.input1(222,"C10H14O","thymol",atomName,atomN);
gd.input2(150.221,323.0,505.7,698.0,0.0,0.0,0.0,0.0,0.0);
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double aCPC222[]={0.0,0.0,0.0,0.0};aCPC=aCPC222;gd.input3(1,aCPC);
double aVPC222[]={0.0,0.0,0.0,0.0};aVPC=aVPC222;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName223[]={"C","H","N"};atomName=atomName223;double atomN223[]={10.0,15.0,1.0};atomN=atomN223;
gd.input1(223,"C10H15N","n-butylaniline",atomName,atomN);
gd.input2(149.236,259.0,513.9,721.0,28.3,0.0,0.0,0.0,0.0);
double aCPC223[]={-34.07,0.9144,-5.56E-4,1.287E-7};aCPC=aCPC223;gd.input3(1,aCPC);
double aVPC223[]={9.7792,4079.72,-96.15,0.0};aVPC=aVPC223;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName224[]={"C","H"};atomName=atomName224;double atomN224[]={10.0,18.0};atomN=atomN224;
gd.input1(224,"C10H18","cis-decalin",atomName,atomN);
gd.input2(138.254,230.0,468.9,702.3,32.0,0.0,0.0,0.286,0.0);
double aCPC224[]={-112.5,1.118,-6.607E-4,1.437E-7};aCPC=aCPC224;gd.input3(1,aCPC);
double aVPC224[]={9.211,3671.61,-69.74,0.0};aVPC=aVPC224;gd.input4(3,aVPC);
gd.input5(-169100.0,85870.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName225[]={"C","H"};atomName=atomName225;double atomN225[]={10.0,18.0};atomN=atomN225;
gd.input1(225,"C10H18","trans-decalin",atomName,atomN);
gd.input2(138.254,242.8,460.5,687.1,31.4,0.0,0.0,0.27,0.0);
double aCPC225[]={-97.67,1.045,-5.476E-4,8.981E-8};aCPC=aCPC225;gd.input3(1,aCPC);
double aVPC225[]={9.1787,3610.66,-66.49,0.0};aVPC=aVPC225;gd.input4(3,aVPC);
gd.input5(-182400.0,73480.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName226[]={"C","H"};atomName=atomName226;double atomN226[]={10.0,18.0};atomN=atomN226;
gd.input1(226,"C10H18","1,3-decadiene",atomName,atomN);
gd.input2(138.254,0.0,442.0,615.0,0.0,0.0,0.0,0.0,0.0);
double aCPC226[]={0.0,0.0,0.0,0.0};aCPC=aCPC226;gd.input3(1,aCPC);
double aVPC226[]={0.0,0.0,0.0,0.0};aVPC=aVPC226;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName227[]={"C","H","N"};atomName=atomName227;double atomN227[]={10.0,19.0,1.0};atomN=atomN227;
gd.input1(227,"C10H19N","caprylonitrile",atomName,atomN);
gd.input2(153.269,255.3,516.0,622.0,32.5,0.0,0.0,0.0,0.0);
double aCPC227[]={0.0,0.0,0.0,0.0};aCPC=aCPC227;gd.input3(1,aCPC);
double aVPC227[]={0.0,0.0,0.0,0.0};aVPC=aVPC227;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName228[]={"C","H"};atomName=atomName228;double atomN228[]={10.0,20.0};atomN=atomN228;
gd.input1(228,"C10H20","butylcyclohexane",atomName,atomN);
gd.input2(140.26,198.4,454.1,667.0,31.5,0.0,0.0,0.362,0.0);
double aCPC228[]={-62.96,1.081,-6.305E-4,1.4E-7};aCPC=aCPC228;gd.input3(1,aCPC);
double aVPC228[]={9.2914,3542.57,-72.32,0.0};aVPC=aVPC228;gd.input4(3,aVPC);
gd.input5(-213300.0,564800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName229[]={"C","H"};atomName=atomName229;double atomN229[]={10.0,20.0};atomN=atomN229;
gd.input1(229,"C10H20","isobutylcyclohexane",atomName,atomN);
gd.input2(140.27,0.0,444.5,659.0,31.2,0.0,0.0,0.319,0.0);
double aCPC229[]={0.0,0.0,0.0,0.0};aCPC=aCPC229;gd.input3(1,aCPC);
double aVPC229[]={-8.05035,2.67134,-5.49473,2.06044};aVPC=aVPC229;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName230[]={"C","H"};atomName=atomName230;double atomN230[]={10.0,20.0};atomN=atomN230;
gd.input1(230,"C10H20","sec-butylcyclohexane",atomName,atomN);
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gd.input2(140.27,0.0,452.5,669.0,26.7,0.0,0.0,0.264,0.0);
double aCPC230[]={0.0,0.0,0.0,0.0};aCPC=aCPC230;gd.input3(1,aCPC);
double aVPC230[]={-7.4925,2.47712,-7.51526,7.69513};aVPC=aVPC230;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName231[]={"C","H"};atomName=atomName231;double atomN231[]={10.0,20.0};atomN=atomN231;
gd.input1(231,"C10H20","tert-butylcyclohexane",atomName,atomN);
gd.input2(140.27,232.0,444.7,659.0,26.6,0.0,0.0,0.525,0.0);
double aCPC231[]={0.0,0.0,0.0,0.0};aCPC=aCPC231;gd.input3(1,aCPC);
double aVPC231[]={-7.34348,2.1381,-6.48025,5.89241};aVPC=aVPC231;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName232[]={"C","H"};atomName=atomName232;double atomN232[]={10.0,20.0};atomN=atomN232;
gd.input1(232,"C10H20","1-decene",atomName,atomN);
gd.input2(140.27,206.9,443.7,615.0,22.0,650.0,0.28,0.491,0.0);
double aCPC232[]={-4.664,0.9077,-5.058E-4,1.095E-7};aCPC=aCPC232;gd.input3(1,aCPC);
double aVPC232[]={-9.05778,3.06154,-7.07236,4.20695};aVPC=aVPC232;gd.input4(1,aVPC);
gd.input5(-124200.0,121100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName233[]={"C","H","O"};atomName=atomName233;double atomN233[]={10.0,20.0,1.0};atomN=atomN233;
gd.input1(233,"C10H20O","menthol",atomName,atomN);
gd.input2(156.269,316.0,489.5,694.0,0.0,0.0,0.0,0.0,0.0);
double aCPC233[]={0.0,0.0,0.0,0.0};aCPC=aCPC233;gd.input3(1,aCPC);
double aVPC233[]={0.0,0.0,0.0,0.0};aVPC=aVPC233;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName234[]={"C","H"};atomName=atomName234;double atomN234[]={10.0,22.0};atomN=atomN234;
gd.input1(234,"C10H22","n-decane",atomName,atomN);
gd.input2(144.286,243.5,447.3,617.7,21.2,603.0,0.249,0.489,0.0);
double aCPC234[]={-7.913,0.9609,-5.288E-4,1.131E-7};aCPC=aCPC234;gd.input3(1,aCPC);
double aVPC234[]={-8.56523,1.97756,-5.81971,-0.29982};aVPC=aVPC234;gd.input4(1,aVPC);
gd.input5(-249800.0,33240.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName235[]={"C","H"};atomName=atomName235;double atomN235[]={10.0,22.0};atomN=atomN235;
gd.input1(235,"C10H22","3,3,5-trimethylheptane",atomName,atomN);
gd.input2(142.286,0.0,428.9,609.7,23.2,0.0,0.0,0.382,0.0);
double aCPC235[]={-70.37,1.232,-8.646E-4,2.455E-7};aCPC=aCPC235;gd.input3(1,aCPC);
double aVPC235[]={9.1646,3305.2,-67.66,0.0};aVPC=aVPC235;gd.input4(3,aVPC);
gd.input5(-258700.0,33580.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName236[]={"C","H"};atomName=atomName236;double atomN236[]={10.0,22.0};atomN=atomN236;
gd.input1(236,"C10H22","2,2,3,3-tetramethylhexane",atomName,atomN);
gd.input2(142.286,0.0,433.5,623.2,25.1,0.0,0.0,0.364,0.0);
double aCPC236[]={-58.83,1.231,-8.834E-4,2.585E-7};aCPC=aCPC236;gd.input3(1,aCPC);
double aVPC236[]={9.1396,3371.05,-64.09,0.0};aVPC=aVPC236;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName237[]={"C","H"};atomName=atomName237;double atomN237[]={10.0,22.0};atomN=atomN237;
gd.input1(237,"C10H22","2,2,5,5-tetramethylhexane",atomName,atomN);
gd.input2(142.286,0.0,410.6,581.6,21.9,0.0,0.0,0.375,0.0);
double aCPC237[]={-62.34,1.245,-8.956E-4,2.618E-7};aCPC=aCPC237;gd.input3(1,aCPC);
double aVPC237[]={9.2244,3172.92,-66.15,0.0};aVPC=aVPC237;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName238[]={"C","H","O"};atomName=atomName238;double atomN238[]={10.0,22.0,1.0};atomN=atomN238;
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gd.input1(238,"C10H22O","1-decanol",atomName,atomN);
gd.input2(158.285,280.1,506.1,687.0,22.2,600.0,0.23,0.0,1.8);
double aCPC238[]={14.57,0.8947,-3.921E-4,3.451E-8};aCPC=aCPC238;gd.input3(1,aCPC);
double aVPC238[]={-8.62283,1.39315,-8.24774,-19.21149};aVPC=aVPC238;gd.input4(1,aVPC);
gd.input5(-401900.0,-104300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName239[]={"C","H","O"};atomName=atomName239;double atomN239[]={11.0,14.0,2.0};atomN=atomN239;
gd.input1(239,"C11H14O2","butylbenzoate",atomName,atomN);
gd.input2(178.232,251.0,523.0,723.0,26.0,561.0,0.25,0.58,0.0);
double aCPC239[]={-17.37,0.8675,-4.61E-4,7.235E-8};aCPC=aCPC239;gd.input3(1,aCPC);
double aVPC239[]={9.7161,4158.47,-94.15,0.0};aVPC=aVPC239;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName240[]={"C","H"};atomName=atomName240;double atomN240[]={11.0,22.0};atomN=atomN240;
gd.input1(240,"C11H22","n-hexylcyclopentane",atomName,atomN);
gd.input2(154.297,200.2,476.3,660.1,21.3,0.0,0.0,0.476,0.0);
double aCPC240[]={-58.32,1.128,-6.536E-4,1.473E-7};aCPC=aCPC240;gd.input3(1,aCPC);
double aVPC240[]={9.3938,3702.56,-81.55,0.0};aVPC=aVPC240;gd.input4(3,aVPC);
gd.input5(-209600.0,78250.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName241[]={"C","H"};atomName=atomName241;double atomN241[]={11.0,22.0};atomN=atomN241;
gd.input1(241,"C11H22","1-undecene",atomName,atomN);
gd.input2(154.297,224.0,465.8,637.0,19.9,0.0,0.0,0.518,0.0);
double aCPC241[]={-5.585,1.003,-5.602E-4,1.216E-7};aCPC=aCPC241;gd.input3(1,aCPC);
double aVPC241[]={71.675,9105.75,-8.489,8596.0};aVPC=aVPC241;gd.input4(2,aVPC);
gd.input5(-144900.0,129500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName242[]={"C","H"};atomName=atomName242;double atomN242[]={11.0,22.0};atomN=atomN242;
gd.input1(242,"C11H24","n-undecane",atomName,atomN);
gd.input2(156.313,247.6,469.1,638.8,19.7,660.0,0.24,0.535,0.0);
double aCPC242[]={-8.395,1.054,-5.799E-4,1.237E-7};aCPC=aCPC242;gd.input3(1,aCPC);
double aVPC242[]={73.501,9305.8,-8.729,8813.0};aVPC=aVPC242;gd.input4(2,aVPC);
gd.input5(-270500.0,41620.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName243[]={"C","H"};atomName=atomName243;double atomN243[]={12.0,10.0};atomN=atomN243;
gd.input1(243,"C12H10","diphenyl",atomName,atomN);
gd.input2(154.212,342.4,529.3,789.0,38.5,502.0,0.295,0.372,0.0);
double aCPC243[]={-97.07,1.106,-8.855E-4,2.79E-7};aCPC=aCPC243;gd.input3(1,aCPC);
double aVPC243[]={-7.674,1.23008,-3.67908,-2.29172};aVPC=aVPC243;gd.input4(1,aVPC);
gd.input5(182200.0,280300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName244[]={"C","H","O"};atomName=atomName244;double atomN244[]={12.0,10.0,1.0};atomN=atomN244;
gd.input1(244,"C12H10O","diphenylether",atomName,atomN);
gd.input2(170.211,300.0,531.2,766.0,31.4,0.0,0.0,0.44,1.1);
double aCPC244[]={-60.73,0.9282,-5.87E-4,1.359E-7};aCPC=aCPC244;gd.input3(1,aCPC);
double aVPC244[]={-8.59849,2.46297,-5.62029,-1.23996};aVPC=aVPC244;gd.input4(1,aVPC);
gd.input5(49990.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName245[]={"C","H"};atomName=atomName245;double atomN245[]={12.0,24.0};atomN=atomN245;
gd.input1(245,"C12H24","n-heptylcyclopentane",atomName,atomN);
gd.input2(168.324,220.0,497.3,679.0,19.4,0.0,0.0,0.515,0.0);
double aCPC245[]={-59.26,1.223,-7.084E-4,1.596E-7};aCPC=aCPC245;gd.input3(1,aCPC);
double aVPC245[]={9.4387,3850.38,-88.75,0.0};aVPC=aVPC245;gd.input4(3,aVPC);
gd.input5(-230300.0,86670.0);
gi.addElement(gd);

gd=new Gas_Data();
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String atomName246[]={"C","H"};atomName=atomName246;double atomN246[]={12.0,24.0};atomN=atomN246;
gd.input1(246,"C12H24","1-dodecene",atomName,atomN);
gd.input2(168.324,238.0,486.5,657.0,18.5,0.0,0.0,0.558,0.0);
double aCPC246[]={-6.544,1.098,-6.155E-4,1.341E-7};aCPC=aCPC246;gd.input3(1,aCPC);
double aVPC246[]={76.348,9846.99,-9.073,9826.0};aVPC=aVPC246;gd.input4(2,aVPC);
gd.input5(-165500.0,138000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName247[]={"C","H"};atomName=atomName247;double atomN247[]={12.0,26.0};atomN=atomN247;
gd.input1(247,"C12H26","dodecane",atomName,atomN);
gd.input2(170.34,263.6,489.5,658.2,18.2,713.0,0.24,0.575,0.0);
double aCPC247[]={-9.328,1.149,-6.347E-4,1.359E-7};aCPC=aCPC247;gd.input3(1,aCPC);
double aVPC247[]={77.628,10012.5,-9.236,10030.0};aVPC=aVPC247;gd.input4(2,aVPC);
gd.input5(-291100.0,50070.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName248[]={"C","H","O"};atomName=atomName248;double atomN248[]={12.0,26.0,1.0};atomN=atomN248;
gd.input1(248,"C12H26O","dihexylether",atomName,atomN);
gd.input2(186.339,230.0,499.6,657.0,18.2,720.0,0.24,0.7,0.0);
double aCPC248[]={33.54,1.073,-5.535E-4,1.678E-7};aCPC=aCPC248;gd.input3(1,aCPC);
double aVPC248[]={9.717,3982.78,-89.15,0.0};aVPC=aVPC248;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName249[]={"C","H","O"};atomName=atomName249;double atomN249[]={12.0,26.0,1.0};atomN=atomN249;
gd.input1(249,"C12H26O","dodecanol",atomName,atomN);
gd.input2(186.339,297.1,533.1,679.0,19.2,718.0,0.24,0.0,1.6);
double aCPC249[]={9.224,1.103,-5.338E-4,7.779E-8};aCPC=aCPC249;gd.input3(1,aCPC);
double aVPC249[]={8.6436,3242.04,-157.1,0.0};aVPC=aVPC249;gd.input4(3,aVPC);
gd.input5(-443100.0,-87130.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName250[]={"C","H","N"};atomName=atomName250;double atomN250[]={12.0,27.0,1.0};atomN=atomN250;
gd.input1(250,"C12H27N","tributylamine",atomName,atomN);
gd.input2(185.355,0.0,486.6,643.0,18.2,0.0,0.0,0.0,0.8);
double aCPC250[]={7.993,1.198,-6.703E-4,1.449E-7};aCPC=aCPC250;gd.input3(1,aCPC);
double aVPC250[]={9.6676,3865.58,-86.15,0.0};aVPC=aVPC250;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName251[]={"C","H"};atomName=atomName251;double atomN251[]={13.0,12.0};atomN=atomN251;
gd.input1(251,"C13H12","diphenylmethane",atomName,atomN);
gd.input2(168.239,300.0,538.2,770.0,28.6,0.0,0.0,0.442,0.4);
double aCPC251[]={0.0,0.0,0.0,0.0};aCPC=aCPC251;gd.input3(1,aCPC);
double aVPC251[]={7.8654,2902.44,-167.9,0.0};aVPC=aVPC251;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName252[]={"C","H"};atomName=atomName252;double atomN252[]={13.0,26.0};atomN=atomN252;
gd.input1(252,"C13H26","n-octylcyclopentane",atomName,atomN);
gd.input2(182.351,229.0,516.9,694.0,17.9,0.0,0.0,0.564,0.0);
double aCPC252[]={-59.95,1.317,-7.612E-4,1.708E-7};aCPC=aCPC252;gd.input3(1,aCPC);
double aVPC252[]={9.4739,3983.01,-95.85,0.0};aVPC=aVPC252;gd.input4(3,aVPC);
gd.input5(-250900.0,91520.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName253[]={"C","H"};atomName=atomName253;double atomN253[]={13.0,26.0};atomN=atomN253;
gd.input1(253,"C13H26","1-tridecene",atomName,atomN);
gd.input2(182.351,250.1,505.9,674.0,17.0,0.0,0.0,0.598,0.0);
double aCPC253[]={-7.118,1.191,-6.674E-4,1.451E-7};aCPC=aCPC253;gd.input3(1,aCPC);
double aVPC253[]={81.389,10609.4,-9.709,11250.0};aVPC=aVPC253;gd.input4(2,aVPC);
gd.input5(-186100.0,146400.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName254[]={"C","H"};atomName=atomName254;double atomN254[]={13.0,28.0};atomN=atomN254;
gd.input1(254,"C13H28","1-tridecane",atomName,atomN);
gd.input2(184.367,267.8,508.6,676.0,17.2,780.0,0.24,0.619,0.0);
double aCPC254[]={-10.46,1.245,-6.912E-4,1.49E-7};aCPC=aCPC254;gd.input3(1,aCPC);
double aVPC254[]={9.5153,3892.91,-98.93,0.0};aVPC=aVPC254;gd.input4(3,aVPC);
gd.input5(-311700.0,58490.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName255[]={"C","H"};atomName=atomName255;double atomN255[]={14.0,10.0};atomN=atomN255;
gd.input1(255,"C14H10","anthracane",atomName,atomN);
gd.input2(178.234,489.7,613.1,869.3,0.0,554.0,0.0,0.0,0.0);
double aCPC255[]={-58.98,1.006,-6.594E-4,1.606E-7};aCPC=aCPC255;gd.input3(1,aCPC);
double aVPC255[]={11.0499,6492.44,-26.13,0.0};aVPC=aVPC255;gd.input4(3,aVPC);
gd.input5(224800.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName256[]={"C","H"};atomName=atomName256;double atomN256[]={14.0,10.0};atomN=atomN256;
gd.input1(256,"C14H10","phenanthrene",atomName,atomN);
gd.input2(178.234,373.7,613.0,873.0,0.0,554.0,0.0,0.0,0.0);
double aCPC256[]={-58.98,1.006,-6.594E-4,1.606E-7};aCPC=aCPC256;gd.input3(1,aCPC);
double aVPC256[]={10.0985,5477.94,-69.39,0.0};aVPC=aVPC256;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName257[]={"C","H"};atomName=atomName257;double atomN257[]={14.0,28.0};atomN=atomN257;
gd.input1(257,"C14H28","n-nonylcyclopentane",atomName,atomN);
gd.input2(196.378,244.0,535.3,710.5,16.5,0.0,0.0,0.61,0.0);
double aCPC257[]={-60.81,1.412,-8.156E-4,1.83E-7};aCPC=aCPC257;gd.input3(1,aCPC);
double aVPC257[]={9.4887,4096.3,-103.0,0.0};aVPC=aVPC257;gd.input4(3,aVPC);
gd.input5(-271500.0,103500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName258[]={"C","H"};atomName=atomName258;double atomN258[]={14.0,28.0};atomN=atomN258;
gd.input1(258,"C14H28","1-tetradecene",atomName,atomN);
gd.input2(196.378,260.3,524.3,689.0,15.6,0.0,0.0,0.644,0.0);
double aCPC258[]={-7.967,1.286,-7.21E-4,1.569E-7};aCPC=aCPC258;gd.input3(1,aCPC);
double aVPC258[]={85.854,11329.2,-10.27,12800.0};aVPC=aVPC258;gd.input4(2,aVPC);
gd.input5(-206700.0,154900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName259[]={"C","H"};atomName=atomName259;double atomN259[]={14.0,30.0};atomN=atomN259;
gd.input1(259,"C14H30","n-tetradecane",atomName,atomN);
gd.input2(198.394,279.0,526.7,693.0,14.4,830.0,0.23,0.581,0.0);
double aCPC259[]={-10.98,1.338,-7.423E-4,1.598E-7};aCPC=aCPC259;gd.input3(1,aCPC);
double aVPC259[]={84.552,11322.9,-10.07,12500.0};aVPC=aVPC259;gd.input4(2,aVPC);
gd.input5(-332300.0,66860.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName260[]={"C","H"};atomName=atomName260;double atomN260[]={15.0,30.0};atomN=atomN260;
gd.input1(260,"C15H30","n-decyclopentane",atomName,atomN);
gd.input2(210.405,251.1,552.5,723.8,15.2,0.0,0.0,0.654,0.0);
double aCPC260[]={-61.92,1.508,-8.717E-4,1.959E-7};aCPC=aCPC260;gd.input3(1,aCPC);
double aVPC260[]={9.5059,4203.94,-109.7,0.0};aVPC=aVPC260;gd.input4(3,aVPC);
gd.input5(-292200.0,111900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName261[]={"C","H"};atomName=atomName261;double atomN261[]={15.0,30.0};atomN=atomN261;
gd.input1(261,"C15H30","1-pentadecene",atomName,atomN);
gd.input2(210.405,269.4,541.5,704.0,14.5,0.0,0.0,0.682,0.0);
double aCPC261[]={-9.203,1.382,-7.783E-4,1.703E-7};aCPC=aCPC261;gd.input3(1,aCPC);
double aVPC261[]={92.3,12205.3,-11.09,14370.0};aVPC=aVPC261;gd.input4(2,aVPC);
gd.input5(-227400.0,163200.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName262[]={"C","H"};atomName=atomName262;double atomN262[]={15.0,32.0};atomN=atomN262;
gd.input1(262,"C15H32","n-pentadecane",atomName,atomN);
gd.input2(212.421,283.0,543.8,707.0,15.2,880.0,0.23,0.706,0.0);
double aCPC262[]={-1.192,1.433,-7.972E-4,1.72E-7};aCPC=aCPC262;gd.input3(1,aCPC);
double aVPC262[]={88.38,11995.6,-10.54,13840.0};aVPC=aVPC262;gd.input4(2,aVPC);
gd.input5(-353000.0,75280.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName263[]={"C","H","O"};atomName=atomName263;double atomN263[]={16.0,22.0,4.0};atomN=atomN263;
gd.input1(263,"C16H22O4","dibutyl-o-phthalate",atomName,atomN);
gd.input2(278.35,238.0,608.0,0.0,0.0,0.0,0.0,0.0,0.0);
double aCPC263[]={1.88,1.254,-6.121E-4,6.971E-8};aCPC=aCPC263;gd.input3(1,aCPC);
double aVPC263[]={10.3337,4852.47,-138.1,0.0};aVPC=aVPC263;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName264[]={"C","H"};atomName=atomName264;double atomN264[]={16.0,32.0};atomN=atomN264;
gd.input1(264,"C16H32","n-decyclohexane",atomName,atomN);
gd.input2(224.432,271.0,570.8,750.0,13.5,0.0,0.0,0.583,0.0);
double aCPC264[]={-69.02,1.654,-9.613E-4,2.143E-7};aCPC=aCPC264;gd.input3(1,aCPC);
double aVPC264[]={9.5425,4373.37,-111.8,0.0};aVPC=aVPC264;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName265[]={"C","H"};atomName=atomName265;double atomN265[]={16.0,32.0};atomN=atomN265;
gd.input1(265,"C16H32","1-hexadecene",atomName,atomN);
gd.input2(224.432,277.3,558.0,717.0,13.3,0.0,0.0,0.721,0.0);
double aCPC265[]={-9.705,1.475,-8.298E-4,1.81E-7};aCPC=aCPC265;gd.input3(1,aCPC);
double aVPC265[]={99.28,13117.0,-11.99,16260.0};aVPC=aVPC265;gd.input4(2,aVPC);
gd.input5(-248000.0,171600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName266[]={"C","H"};atomName=atomName266;double atomN266[]={16.0,34.0};atomN=atomN266;
gd.input1(266,"C16H34","hexadecane",atomName,atomN);
gd.input2(226.448,291.0,560.0,722.0,14.1,0.0,0.0,0.742,0.0);
double aCPC266[]={-13.02,1.529,-8.537E-4,1.85E-7};aCPC=aCPC266;gd.input3(1,aCPC);
double aVPC266[]={89.06,12411.3,-10.58,15200.0};aVPC=aVPC266;gd.input4(2,aVPC);
gd.input5(-373600.0,83740.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName267[]={"C","H"};atomName=atomName267;double atomN267[]={17.0,34.0};atomN=atomN267;
gd.input1(267,"C17H34","n-dodecyclopentane",atomName,atomN);
gd.input2(238.459,268.0,584.1,750.0,12.9,0.0,0.0,0.719,0.0);
double aCPC267[]={-63.26,1.695,-9.768E-4,2.186E-7};aCPC=aCPC267;gd.input3(1,aCPC);
double aVPC267[]={9.5713,4395.87,-124.2,0.0};aVPC=aVPC267;gd.input4(3,aVPC);
gd.input5(-336100.0,126000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName268[]={"C","H","O"};atomName=atomName268;double atomN268[]={17.0,36.0,1.0};atomN=atomN268;
gd.input1(268,"C17H36O","heptadecanol",atomName,atomN);
gd.input2(256.474,327.0,597.0,736.0,14.1,0.0,0.0,0.0,0.0);
double aCPC268[]={-7.792,1.653,-9.345E-4,2.044E-7};aCPC=aCPC268;gd.input3(1,aCPC);
double aVPC268[]={8.9959,3672.62,-188.1,0.0};aVPC=aVPC268;gd.input4(3,aVPC);
gd.input5(-546300.0,-44670.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName269[]={"C","H"};atomName=atomName269;double atomN269[]={18.0,14.0};atomN=atomN269;
gd.input1(269,"C18H14","o-terphenyl",atomName,atomN);
gd.input2(230.31,330.0,605.0,891.0,39.0,753.0,0.396,0.431,0.0);
double aCPC269[]={0.0,0.0,0.0,0.0};aCPC=aCPC269;gd.input3(1,aCPC);
double aVPC269[]={0.0,0.0,0.0,0.0};aVPC=aVPC269;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName270[]={"C","H"};atomName=atomName270;double atomN270[]={18.0,14.0};atomN=atomN270;
gd.input1(270,"C18H14","m-terphenyl",atomName,atomN);
gd.input2(230.31,360.0,638.0,924.9,35.1,768.0,0.358,0.449,0.0);
double aCPC270[]={0.0,0.0,0.0,0.0};aCPC=aCPC270;gd.input3(1,aCPC);
double aVPC270[]={0.0,0.0,0.0,0.0};aVPC=aVPC270;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName271[]={"C","H"};atomName=atomName271;double atomN271[]={18.0,14.0};atomN=atomN271;
gd.input1(271,"C18H14","p-terphenyl",atomName,atomN);
gd.input2(230.31,485.0,649.0,926.0,33.2,763.0,0.329,0.523,0.7);
double aCPC271[]={0.0,0.0,0.0,0.0};aCPC=aCPC271;gd.input3(1,aCPC);
double aVPC271[]={0.0,0.0,0.0,0.0};aVPC=aVPC271;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName272[]={"C","H"};atomName=atomName272;double atomN272[]={18.0,36.0};atomN=atomN272;
gd.input1(272,"C18H36","1-octadecene",atomName,atomN);
gd.input2(252.486,290.8,588.0,739.0,11.3,0.0,0.0,0.807,0.0);
double aCPC272[]={-11.33,1.664,-9.374E-4,2.049E-7};aCPC=aCPC272;gd.input3(1,aCPC);
double aVPC272[]={9.6019,4416.13,-127.3,0.0};aVPC=aVPC272;gd.input4(3,aVPC);
gd.input5(-289200.0,188400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName273[]={"C","H"};atomName=atomName273;double atomN273[]={18.0,36.0};atomN=atomN273;
gd.input1(273,"C18H36","n-tridecyclopentane",atomName,atomN);
gd.input2(252.486,278.0,598.6,761.0,12.0,0.0,0.0,0.755,0.0);
double aCPC273[]={-64.21,1.79,-0.001032,2.309E-7};aCPC=aCPC273;gd.input3(1,aCPC);
double aVPC273[]={9.6068,4483.13,-131.3,0.0};aVPC=aVPC273;gd.input4(3,aVPC);
gd.input5(-354000.0,137100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName274[]={"C","H"};atomName=atomName274;double atomN274[]={18.0,38.0};atomN=atomN274;
gd.input1(274,"C18H38","octadecane",atomName,atomN);
gd.input2(254.504,301.3,589.5,748.0,12.0,0.0,0.0,0.79,0.0);
double aCPC274[]={-14.47,1.717,-9.592E-4,2.078E-7};aCPC=aCPC274;gd.input3(1,aCPC);
double aVPC274[]={9.503,4361.79,-129.9,0.0};aVPC=aVPC274;gd.input4(3,aVPC);
gd.input5(-414800.0,100600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName275[]={"C","H","O"};atomName=atomName275;double atomN275[]={18.0,38.0,1.0};atomN=atomN275;
gd.input1(275,"C18H38O","1-octadecanol",atomName,atomN);
gd.input2(270.501,331.0,608.0,747.0,14.1,0.0,0.0,0.0,1.7);
double aCPC275[]={-8.704,1.748,-9.881E-4,2.157E-7};aCPC=aCPC275;gd.input3(1,aCPC);
double aVPC275[]={9.0696,3757.82,-193.1,0.0};aVPC=aVPC275;gd.input4(3,aVPC);
gd.input5(-566900.0,-36220.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName276[]={"C","H"};atomName=atomName276;double atomN276[]={19.0,38.0};atomN=atomN276;
gd.input1(276,"C19H38","1-cyclopentyltetradecane",atomName,atomN);
gd.input2(266.513,282.0,599.0,772.0,11.2,0.0,0.0,0.789,0.0);
double aCPC276[]={-64.93,1.884,-0.001085,2.426E-7};aCPC=aCPC276;gd.input3(1,aCPC);
double aVPC276[]={9.643,4439.38,-138.1,0.0};aVPC=aVPC276;gd.input4(3,aVPC);
gd.input5(-374600.0,145600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName277[]={"C","H"};atomName=atomName277;double atomN277[]={19.0,40.0};atomN=atomN277;
gd.input1(277,"C19H40","n-nonadecane",atomName,atomN);
gd.input2(268.529,305.0,603.1,756.0,11.1,0.0,0.0,0.827,0.0);
double aCPC277[]={-15.49,1.812,-0.001015,2.205E-7};aCPC=aCPC277;gd.input3(1,aCPC);
double aVPC277[]={9.5331,4450.44,-135.6,0.0};aVPC=aVPC277;gd.input4(3,aVPC);
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gd.input5(-435400.0,109000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName278[]={"C","H"};atomName=atomName278;double atomN278[]={20.0,40.0};atomN=atomN278;
gd.input1(278,"C20H40","1-cyclopentylpentadecane",atomName,atomN);
gd.input2(280.54,290.0,625.0,780.0,10.2,0.0,0.0,0.833,0.0);
double aCPC278[]={-66.09,1.98,-0.00114,2.55E-7};aCPC=aCPC278;gd.input3(1,aCPC);
double aVPC278[]={9.689,4692.01,-145.1,0.0};aVPC=aVPC278;gd.input4(3,aVPC);
gd.input5(-395300.0,154000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName279[]={"C","H","O"};atomName=atomName279;double atomN279[]={20.0,42.0,1.0};atomN=atomN279;
gd.input1(279,"C20H42O","1-eicosanol",atomName,atomN);
gd.input2(298.555,339.0,629.0,770.0,12.0,0.0,0.0,0.0,0.0);
double aCPC279[]={-12.58,1.95,-0.001118,2.516E-7};aCPC=aCPC279;gd.input3(1,aCPC);
double aVPC279[]={9.2031,3912.1,-203.1,0.0};aVPC=aVPC279;gd.input4(3,aVPC);
gd.input5(-608100.0,-19430.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName280[]={"C","F"};atomName=atomName280;double atomN280[]={6.0,6.0};atomN=atomN280;
gd.input1(280,"C6F6","perfluorobenzene",atomName,atomN);
gd.input2(186.056,0.0,353.4,516.7,33.0,335.0,0.255,0.396,0.0);
double aCPC280[]={36.28,0.5267,-4.547E-4,1.456E-7};aCPC=aCPC280;gd.input3(1,aCPC);
double aVPC280[]={7.97271,1.43798,-3.62195,-4.79241};aVPC=aVPC280;gd.input4(1,aVPC);
gd.input5(-957300.0,-880000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName281[]={"C","F"};atomName=atomName281;double atomN281[]={6.0,12.0};atomN=atomN281;
gd.input1(281,"C6F12","perfluorocyclohexane",atomName,atomN);
gd.input2(300.047,0.0,326.0,457.2,24.3,459.0,0.27,0.432,0.0);
double aCPC281[]={0.0,0.0,0.0,0.0};aCPC=aCPC281;gd.input3(1,aCPC);
double aVPC281[]={7.2885,1374.07,-136.8,0.0};aVPC=aVPC281;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName282[]={"C","F"};atomName=atomName282;double atomN282[]={6.0,14.0};atomN=atomN282;
gd.input1(282,"C6F14","perfluoro-n-hexane",atomName,atomN);
gd.input2(338.044,186.0,329.8,448.8,18.7,606.0,0.303,0.514,0.0);
double aCPC282[]={0.0,0.0,0.0,0.0};aCPC=aCPC282;gd.input3(1,aCPC);
double aVPC282[]={-9.16184,2.97539,-7.17322,5.50684};aVPC=aVPC282;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName283[]={"C","F"};atomName=atomName283;double atomN283[]={6.0,14.0};atomN=atomN283;
gd.input1(283,"C6F14","perfluoro-2-methylpentane",atomName,atomN);
gd.input2(338.044,0.0,330.8,453.0,18.2,550.0,0.266,0.464,0.0);
double aCPC283[]={0.0,0.0,0.0,0.0};aCPC=aCPC283;gd.input3(1,aCPC);
double aVPC283[]={9.6896,2760.0,-45.7,0.0};aVPC=aVPC283;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName284[]={"C","F"};atomName=atomName284;double atomN284[]={6.0,14.0};atomN=atomN284;
gd.input1(284,"C6F14","perfluoro-3-methylpentane",atomName,atomN);
gd.input2(338.044,0.0,331.5,450.0,16.9,0.0,0.0,0.476,0.0);
double aCPC284[]={0.0,0.0,0.0,0.0};aCPC=aCPC284;gd.input3(1,aCPC);
double aVPC284[]={9.267,2565.44,-54.23,0.0};aVPC=aVPC284;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName285[]={"C","F"};atomName=atomName285;double atomN285[]={6.0,14.0};atomN=atomN285;
gd.input1(285,"C6F14","perfluoro-2,3-dimethylbutane",atomName,atomN);
gd.input2(338.044,0.0,332.9,463.0,18.7,525.0,0.256,0.394,0.0);
double aCPC285[]={0.0,0.0,0.0,0.0};aCPC=aCPC285;gd.input3(1,aCPC);
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double aVPC285[]={9.9846,2933.85,-38.7,0.0};aVPC=aVPC285;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName286[]={"C","H","F"};atomName=atomName286;double atomN286[]={6.0,1.0,5.0};atomN=atomN286;
gd.input1(286,"C6HF5","pentafluorobenzene",atomName,atomN);
gd.input2(168.064,0.0,358.9,531.0,35.3,324.0,0.26,0.373,0.0);
double aCPC286[]={0.0,0.0,0.0,0.0};aCPC=aCPC286;gd.input3(1,aCPC);
double aVPC286[]={-7.7973,1.35271,-3.50409,-3.76856};aVPC=aVPC286;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName287[]={"C","H","F","O"};atomName=atomName287;double atomN287[]={6.0,1.0,5.0,1.0};atomN=atomN287;
gd.input1(287,"C6HF5O","pentafluorophenol",atomName,atomN);
gd.input2(184.063,0.0,418.8,609.0,40.0,348.0,0.275,0.502,0.0);
double aCPC287[]={0.0,0.0,0.0,0.0};aCPC=aCPC287;gd.input3(1,aCPC);
double aVPC287[]={-8.69734,2.03071,-5.32619,-3.28915};aVPC=aVPC287;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName288[]={"C","H","F"};atomName=atomName288;double atomN288[]={6.0,2.0,4.0};atomN=atomN288;
gd.input1(288,"C6H2F4","1,2,3,4-tetrafluorobenzene",atomName,atomN);
gd.input2(150.074,0.0,367.5,550.8,37.9,313.0,0.259,0.344,0.0);
double aCPC288[]={0.0,0.0,0.0,0.0};aCPC=aCPC288;gd.input3(1,aCPC);
double aVPC288[]={-7.71223,1.48262,-3.55669,-2.83189};aVPC=aVPC288;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName289[]={"C","H","F"};atomName=atomName289;double atomN289[]={6.0,2.0,4.0};atomN=atomN289;
gd.input1(289,"C6H2F4","1,2,3,5-tetrafluorobenzene",atomName,atomN);
gd.input2(150.074,0.0,357.6,535.5,37.5,0.0,0.0,0.346,0.0);
double aCPC289[]={0.0,0.0,0.0,0.0};aCPC=aCPC289;gd.input3(1,aCPC);
double aVPC289[]={-7.71193,1.46356,-3.49452,-3.04916};aVPC=aVPC289;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName290[]={"C","H","F"};atomName=atomName290;double atomN290[]={6.0,2.0,4.0};atomN=atomN290;
gd.input1(290,"C6H2F4","1,2,4,5-tetrafluorobenzene",atomName,atomN);
gd.input2(150.074,0.0,363.4,543.4,38.0,0.0,0.0,0.355,0.0);
double aCPC290[]={0.0,0.0,0.0,0.0};aCPC=aCPC290;gd.input3(1,aCPC);
double aVPC290[]={-7.7974,1.57406,-3.8206,-2.45398};aVPC=aVPC290;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName291[]={"C","H","Cl"};atomName=atomName291;double atomN291[]={6.0,4.0,2.0};atomN=atomN291;
gd.input1(291,"C6H4Cl2","o-dichlorobenzene",atomName,atomN);
gd.input2(147.004,256.1,452.0,729.0,41.0,360.0,0.244,0.272,2.3);
double aCPC291[]={-14.3,0.5506,-4.513E-4,1.429E-7};aCPC=aCPC291;gd.input3(1,aCPC);
double aVPC291[]={-8.23991,6.34949,-13.24326,17.25417};aVPC=aVPC291;gd.input4(1,aVPC);
gd.input5(30000.0,82730.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName292[]={"C","H","F"};atomName=atomName292;double atomN292[]={6.0,4.0,2.0};atomN=atomN292;
gd.input1(292,"C6H4F2","1,4-difluorobenzene",atomName,atomN);
gd.input2(114.094,0.0,362.0,556.0,44.0,0.0,0.0,0.299,0.0);
double aCPC292[]={-25.96,0.5722,-4.677E-4,1.475E-7};aCPC=aCPC292;gd.input3(1,aCPC);
double aVPC292[]={0.0,0.0,0.0,0.0};aVPC=aVPC292;gd.input4(0,aVPC);
gd.input5(-307400.0,-253000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName293[]={"C","H","Br"};atomName=atomName293;double atomN293[]={6.0,5.0,1.0};atomN=atomN293;
gd.input1(293,"C6H5Br","bromobenzene",atomName,atomN);
gd.input2(157.01,242.3,429.2,670.0,45.2,324.0,0.263,0.251,1.5);
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double aCPC293[]={-28.81,0.5351,-4.08E-4,1.212E-7};aCPC=aCPC293;gd.input3(1,aCPC);
double aVPC293[]={-7.54985,2.09359,-3.57864,-1.82558};aVPC=aVPC293;gd.input4(1,aVPC);
gd.input5(105100.0,138600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName294[]={"C","H","F"};atomName=atomName294;double atomN294[]={6.0,5.0,1.0};atomN=atomN294;
gd.input1(294,"C6H5F","fluorobenzene",atomName,atomN);
gd.input2(96.104,234.0,357.9,560.1,45.5,269.0,0.263,0.244,1.4);
double aCPC294[]={-38.73,0.5669,-4.434E-4,1.355E-7};aCPC=aCPC294;gd.input3(1,aCPC);
double aVPC294[]={48.521,5819.21,-5.489,2910.0};aVPC=aVPC294;gd.input4(2,aVPC);
gd.input5(-116600.0,-69080.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName295[]={"C","H","I"};atomName=atomName295;double atomN295[]={6.0,5.0,1.0};atomN=atomN295;
gd.input1(295,"C6H5I","iodobenzene",atomName,atomN);
gd.input2(204.011,241.8,461.6,721.0,45.2,351.0,0.265,0.249,1.4);
double aCPC295[]={-29.27,0.5564,-4.509E-4,1.443E-7};aCPC=aCPC295;gd.input3(1,aCPC);
double aVPC295[]={51.071,7589.5,-5.646,4845.0};aVPC=aVPC295;gd.input4(2,aVPC);
gd.input5(162700.0,187900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName296[]={"C","H"};atomName=atomName296;double atomN296[]={6.0,6.0};atomN=atomN296;
gd.input1(296,"C6H6","benzene",atomName,atomN);
gd.input2(78.114,278.7,353.2,562.2,48.9,259.0,0.271,0.212,0.0);
double aCPC296[]={-33.92,0.4739,-3.017E-4,7.13E-8};aCPC=aCPC296;gd.input3(1,aCPC);
double aVPC296[]={-6.98273,1.33213,-2.62863,-3.33399};aVPC=aVPC296;gd.input4(1,aVPC);
gd.input5(82980.0,129700.0);
double agC6H14[][]={{-47.65775134130275,460.81434893807244,6.008223493326193,-163.4612548550745,200.0,275.0},
{-74.35657484909136,595.6242224122708,9.127577432603973,-355.1790365035916,275.0,350.0},
{-67.20605604300314,569.8326515784917,7.506819988190337,-329.05986681020033,350.0,425.0},
{-39.45768448032993,483.15547377393005,-0.9470035741110165,-252.8259758887665,425.0,500.0},
{-0.10216607547920376,378.18690139312986,-17.37943171586526,-174.01901971669156,500.0,575.0},
{42.27205421616631,279.723927495227,-40.676585243570365,-109.6307014017849,575.0,650.0},
{78.17762568209508,205.76728183593355,-65.78877439192944,-66.76688691516311,650.0,725.0},
{96.70301336612965,171.33104431157534,-81.68810921854958,-48.75836706771078,725.0,800.0},
{85.27046744340731,189.97599751359974,-68.95793254594496,-57.309158856043936,800.0,875.0},
{29.51591096933322,274.4945907867724,2.982998166113406,-93.3523642096161,875.0,950.0},
{-879.4704585808074,1521.4510564554264,1433.7095349172425,-574.4066899473296,950.0,1100.0},
{351.26851875076744,-124.30964716853704,-629.8572246234078,45.542619806297026,1100.0,1500.0}};
gi.addElement(gd);
gd.inputCp(agC6H14);

gd=new Gas_Data();
String atomName297[]={"C","H","O"};atomName=atomName297;double atomN297[]={6.0,6.0,1.0};atomN=atomN297;
gd.input1(297,"C6H6O","phenol",atomName,atomN);
gd.input2(94.113,314.0,455.0,694.2,61.3,229.0,0.24,0.438,1.6);
double aCPC297[]={-35.84,0.5983,-4.827E-4,1.527E-7};aCPC=aCPC297;gd.input3(1,aCPC);
double aVPC297[]={-8.7555,2.92651,-6.31601,-1.36889};aVPC=aVPC297;gd.input4(1,aVPC);
gd.input5(-96420.0,-32900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName298[]={"C","H","N"};atomName=atomName298;double atomN298[]={6.0,7.0,1.0};atomN=atomN298;
gd.input1(298,"C6H7N","aniline",atomName,atomN);
gd.input2(93.129,267.0,457.6,699.0,53.1,274.0,0.25,0.384,1.6);
double aCPC298[]={-40.52,0.6385,-5.133E-4,1.633E-7};aCPC=aCPC298;gd.input3(1,aCPC);
double aVPC298[]={-7.65517,0.85386,-2.51602,-5.96795};aVPC=aVPC298;gd.input4(1,aVPC);
gd.input5(86920.0,166800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName299[]={"C","H","N"};atomName=atomName299;double atomN299[]={6.0,7.0,1.0};atomN=atomN299;
gd.input1(299,"C6H7N","2-methylpyridine",atomName,atomN);
gd.input2(93.129,207.0,402.6,621.0,46.0,0.0,0.0,0.299,1.9);
double aCPC299[]={-36.26,0.5584,-3.704E-4,9.663E-8};aCPC=aCPC299;gd.input3(1,aCPC);
double aVPC299[]={9.5725,3259.83,-61.58,0.0};aVPC=aVPC299;gd.input4(3,aVPC);
gd.input5(99020.0,177200.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName300[]={"C","H","N"};atomName=atomName300;double atomN300[]={6.0,7.0,1.0};atomN=atomN300;
gd.input1(300,"C6H7N","3-methylpyridine",atomName,atomN);
gd.input2(93.129,0.0,417.3,645.0,0.0,0.0,0.0,0.0,2.4);
double aCPC300[]={-37.09,0.56,-3.719E-4,9.685E-8};aCPC=aCPC300;gd.input3(1,aCPC);
double aVPC300[]={9.6136,3411.91,-61.95,0.0};aVPC=aVPC300;gd.input4(3,aVPC);
gd.input5(106200.0,184400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName301[]={"C","H","N"};atomName=atomName301;double atomN301[]={6.0,7.0,1.0};atomN=atomN301;
gd.input1(301,"C6H7N","4-methylpyridine",atomName,atomN);
gd.input2(93.129,276.9,418.5,646.0,44.6,311.0,0.26,0.301,0.0);
double aCPC301[]={-17.43,0.4882,-2.798E-4,5.451E-8};aCPC=aCPC301;gd.input3(1,aCPC);
double aVPC301[]={-7.13732,0.93444,-2.93708,-2.65045};aVPC=aVPC301;gd.input4(1,aVPC);
gd.input5(102300.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName302[]={"C","H"};atomName=atomName302;double atomN302[]={6.0,10.0};atomN=atomN302;
gd.input1(302,"C6H10","1,5-hexadiene",atomName,atomN);
gd.input2(82.146,132.0,332.6,507.0,34.4,0.0,0.0,0.16,0.0);
double aCPC302[]={0.0,0.0,0.0,0.0};aCPC=aCPC302;gd.input3(1,aCPC);
double aVPC302[]={-7.72848,2.21648,-2.2319,-8.51382};aVPC=aVPC302;gd.input4(1,aVPC);
gd.input5(83740.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName303[]={"C","H"};atomName=atomName303;double atomN303[]={6.0,10.0};atomN=atomN303;
gd.input1(303,"C6H10","cyclohexene",atomName,atomN);
gd.input2(82.146,169.7,356.1,560.5,43.4,0.0,0.0,0.21,0.6);
double aCPC303[]={-68.65,0.7252,-5.414E-4,1.644E-7};aCPC=aCPC303;gd.input3(1,aCPC);
double aVPC303[]={9.2041,2813.53,-49.98,0.0};aVPC=aVPC303;gd.input4(3,aVPC);
gd.input5(-5360.0,106900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName304[]={"C","H","O"};atomName=atomName304;double atomN304[]={5.0,12.0,1.0};atomN=atomN304;
gd.input1(304,"C5H12O","2,2-dimethyl-1-propanol",atomName,atomN);
gd.input2(88.15,327.0,386.3,549.0,0.0,0.0,0.0,0.0,0.0);
double aCPC304[]={12.15,0.5397,-3.16E-4,7.122E-8};aCPC=aCPC304;gd.input3(1,aCPC);
double aVPC304[]={11.5134,3694.96,-65.0,0.0};aVPC=aVPC304;gd.input4(3,aVPC);
gd.input5(-293100.0,-125500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName305[]={"C","H","O"};atomName=atomName305;double atomN305[]={5.0,12.0,1.0};atomN=atomN305;
gd.input1(305,"C5H12O","ethylpropylether",atomName,atomN);
gd.input2(88.15,146.4,336.4,500.2,33.7,339.0,0.275,0.333,1.2);
double aCPC305[]={0.0,0.0,0.0,0.0};aCPC=aCPC305;gd.input3(1,aCPC);
double aVPC305[]={-8.0582,2.35916,-4.51822,0.92352};aVPC=aVPC305;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName306[]={"C","H","O"};atomName=atomName306;double atomN306[]={5.0,12.0,1.0};atomN=atomN306;
gd.input1(306,"C5H12O","butylmethylether",atomName,atomN);
gd.input2(88.15,157.7,343.3,512.8,33.7,329.0,0.26,0.316,1.3);
double aCPC306[]={0.0,0.0,0.0,0.0};aCPC=aCPC306;gd.input3(1,aCPC);
double aVPC306[]={-7.7511,1.87213,-3.80629,-1.8141};aVPC=aVPC306;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName307[]={"C","H","O"};atomName=atomName307;double atomN307[]={5.0,12.0,1.0};atomN=atomN307;
gd.input1(307,"C5H12O","tert-butylmethylether",atomName,atomN);
gd.input2(88.15,0.0,328.3,496.4,33.7,0.0,0.0,0.269,1.2);
double aCPC307[]={2.534,0.5136,-2.596E-4,4.303E-8};aCPC=aCPC307;gd.input3(1,aCPC);
double aVPC307[]={-7.82516,2.95493,-6.94079,12.17416};aVPC=aVPC307;gd.input4(1,aVPC);
gd.input5(-293100.0,-125500.0);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName308[]={"C","Br","F"};atomName=atomName308;double atomN308[]={6.0,1.0,5.0};atomN=atomN308;
gd.input1(308,"C6BrF5","bromopentafluorobenzene",atomName,atomN);
gd.input2(246.96,0.0,410.0,601.0,30.4,0.0,0.0,0.355,0.0);
double aCPC308[]={0.0,0.0,0.0,0.0};aCPC=aCPC308;gd.input3(1,aCPC);
double aVPC308[]={0.0,0.0,0.0,0.0};aVPC=aVPC308;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName309[]={"C","Cl","F"};atomName=atomName309;double atomN309[]={6.0,1.0,5.0};atomN=atomN309;
gd.input1(309,"C6ClF5","chloropentafluorobenzene",atomName,atomN);
gd.input2(202.509,0.0,391.1,570.8,32.4,376.0,0.256,0.4,0.0);
double aCPC309[]={0.0,0.0,0.0,0.0};aCPC=aCPC309;gd.input3(1,aCPC);
double aVPC309[]={-8.02172,1.54665,-3.78361,-2.99849};aVPC=aVPC309;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName310[]={"C","Cl","F"};atomName=atomName310;double atomN310[]={6.0,2.0,4.0};atomN=atomN310;
gd.input1(310,"C6Cl2F4","dichlorotetrafluorobenzene",atomName,atomN);
gd.input2(218.964,0.0,430.9,626.0,53.2,0.0,0.0,0.622,0.0);
double aCPC310[]={0.0,0.0,0.0,0.0};aCPC=aCPC310;gd.input3(1,aCPC);
double aVPC310[]={0.0,0.0,0.0,0.0};aVPC=aVPC310;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName311[]={"C","Cl","F"};atomName=atomName311;double atomN311[]={6.0,3.0,3.0};atomN=atomN311;
gd.input1(311,"C6Cl3F3","1,3,5-trichlorotrifluorobenzene",atomName,atomN);
gd.input2(235.419,0.0,471.5,684.9,32.7,448.0,0.257,0.426,0.0);
double aCPC311[]={0.0,0.0,0.0,0.0};aCPC=aCPC311;gd.input3(1,aCPC);
double aVPC311[]={-8.2094,1.6886,-4.17824,-1.54115};aVPC=aVPC311;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName312[]={"C","H","N"};atomName=atomName312;double atomN312[]={3.0,9.0,1.0};atomN=atomN312;
gd.input1(312,"C3H9N","n-propylamine",atomName,atomN);
gd.input2(59.112,190.0,321.7,497.0,48.1,233.0,0.271,0.303,1.3);
double aCPC312[]={6.691,0.3498,-1.822E-4,3.586E-8};aCPC=aCPC312;gd.input3(1,aCPC);
double aVPC312[]={-7.23587,1.22853,-3.75004,-4.3399};aVPC=aVPC312;gd.input4(1,aVPC);
gd.input5(-72430.0,39820.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName313[]={"C","H","N"};atomName=atomName313;double atomN313[]={3.0,9.0,1.0};atomN=atomN313;
gd.input1(313,"C3H9N","isopropylamine",atomName,atomN);
gd.input2(59.112,177.9,305.6,471.8,45.4,221.0,0.225,0.291,0.0);
double aCPC313[]={-7.486,0.4175,-2.826E-4,8.348E-8};aCPC=aCPC313;gd.input3(1,aCPC);
double aVPC313[]={-7.40866,1.79229,-4.75675,-1.70138};aVPC=aVPC313;gd.input4(1,aVPC);
gd.input5(-83820.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName314[]={"C","H","N"};atomName=atomName314;double atomN314[]={3.0,9.0,1.0};atomN=atomN314;
gd.input1(314,"C3H9N","trimethylamine",atomName,atomN);
gd.input2(59.112,156.0,276.0,433.3,40.9,254.0,0.288,0.205,0.6);
double aCPC314[]={-8.206,0.3972,-2.219E-4,4.622E-8};aCPC=aCPC314;gd.input3(1,aCPC);
double aVPC314[]={-6.88066,1.15962,-2.18332,-2.94707};aVPC=aVPC314;gd.input4(1,aVPC);
gd.input5(-23860.0,98980.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName315[]={"C","F"};atomName=atomName315;double atomN315[]={4.0,8.0};atomN=atomN315;
gd.input1(315,"C4F8","perfluorocyclobutane",atomName,atomN);
gd.input2(200.028,0.0,267.2,388.5,27.8,324.0,0.279,0.356,0.0);
double aCPC315[]={0.0,0.0,0.0,0.0};aCPC=aCPC315;gd.input3(1,aCPC);
double aVPC315[]={9.0726,1985.95,-48.01,0.0};aVPC=aVPC315;gd.input4(3,aVPC);
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gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName316[]={"C","F"};atomName=atomName316;double atomN316[]={4.0,10.0};atomN=atomN316;
gd.input1(316,"C4F10","perfluorobutane",atomName,atomN);
gd.input2(238.024,145.0,271.2,386.4,23.2,378.0,0.274,0.374,0.0);
double aCPC316[]={0.0,0.0,0.0,0.0};aCPC=aCPC316;gd.input3(1,aCPC);
double aVPC316[]={9.5788,2280.18,-32.82,0.0};aVPC=aVPC316;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName317[]={"C","H"};atomName=atomName317;double atomN317[]={4.0,4.0};atomN=atomN317;
gd.input1(317,"C4H4","vinylacetylene",atomName,atomN);
gd.input2(52.076,227.6,278.1,455.0,49.6,202.0,0.26,0.092,0.0);
double aCPC317[]={6.757,0.2841,-2.265E-4,7.461E-8};aCPC=aCPC317;gd.input3(1,aCPC);
double aVPC317[]={9.3898,2203.57,-43.15,0.0};aVPC=aVPC317;gd.input4(3,aVPC);
gd.input5(304800.0,306200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName318[]={"C","H","O"};atomName=atomName318;double atomN318[]={4.0,4.0,1.0};atomN=atomN318;
gd.input1(318,"C4H4O","furan",atomName,atomN);
gd.input2(68.075,187.5,304.5,490.2,55.0,218.0,0.295,0.209,0.7);
double aCPC318[]={-35.53,0.4321,-3.455E-4,1.047E-7};aCPC=aCPC318;gd.input3(1,aCPC);
double aVPC318[]={9.441,2442.7,-45.41,0.0};aVPC=aVPC318;gd.input4(3,aVPC);
gd.input5(-34700.0,879.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName319[]={"C","H","N"};atomName=atomName319;double atomN319[]={4.0,4.0,1.0};atomN=atomN319;
gd.input1(319,"C4H4N","thiophene",atomName,atomN);
gd.input2(84.136,234.9,357.2,579.4,56.9,219.0,0.258,0.196,0.5);
double aCPC319[]={-30.61,0.448,-3.772E-4,1.253E-7};aCPC=aCPC319;gd.input3(1,aCPC);
double aVPC319[]={-7.05208,1.6964,-3.17778,-1.157742};aVPC=aVPC319;gd.input4(1,aVPC);
gd.input5(115800.0,126900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName320[]={"C","H","N"};atomName=atomName320;double atomN320[]={4.0,5.0,1.0};atomN=atomN320;
gd.input1(320,"C4H5N","allylcyanide",atomName,atomN);
gd.input2(67.091,186.7,392.0,585.0,39.5,265.0,0.22,0.39,3.4);
double aCPC320[]={21.7,0.2572,-1.192E-4,1.229E-8};aCPC=aCPC320;gd.input3(1,aCPC);
double aVPC320[]={9.3817,3128.75,-58.15,0.0};aVPC=aVPC320;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName321[]={"C","H","N"};atomName=atomName321;double atomN321[]={4.0,5.0,1.0};atomN=atomN321;
gd.input1(321,"C4H5N","pyrrole",atomName,atomN);
gd.input2(67.091,0.0,403.0,639.8,0.0,0.0,0.0,0.0,1.8);
double aCPC321[]={0.0,0.0,0.0,0.0};aCPC=aCPC321;gd.input3(1,aCPC);
double aVPC321[]={10.1764,3457.47,-62.73,0.0};aVPC=aVPC321;gd.input4(3,aVPC);
gd.input5(108400.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName322[]={"C","H"};atomName=atomName322;double atomN322[]={4.0,6.0};atomN=atomN322;
gd.input1(322,"C4H6","1-butyne",atomName,atomN);
gd.input2(54.092,147.4,281.2,463.7,47.1,220.0,0.27,0.05,0.8);
double aCPC322[]={12.55,0.2744,-1.545E-4,3.45E-8};aCPC=aCPC322;gd.input3(1,aCPC);
double aVPC322[]={-6.29693,2.12358,-6.42124,4.11543};aVPC=aVPC322;gd.input4(1,aVPC);
gd.input5(165300.0,202200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName323[]={"C","H"};atomName=atomName323;double atomN323[]={4.0,6.0};atomN=atomN323;
gd.input1(323,"C4H6","2-butyne",atomName,atomN);
gd.input2(54.092,240.9,300.1,488.7,50.8,221.0,0.277,0.124,0.8);
double aCPC323[]={15.93,0.2381,-1.07E-4,1.753E-8};aCPC=aCPC323;gd.input3(1,aCPC);
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double aVPC323[]={9.6669,2536.78,-37.34,0.0};aVPC=aVPC323;gd.input4(3,aVPC);
gd.input5(146400.0,185600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName324[]={"C","H"};atomName=atomName324;double atomN324[]={4.0,6.0};atomN=atomN324;
gd.input1(324,"C4H6","1,2-butadiene",atomName,atomN);
gd.input2(54.092,137.0,284.0,443.7,44.9,219.0,0.267,0.255,0.4);
double aCPC324[]={11.2,0.2724,-1.468E-4,3.089E-8};aCPC=aCPC324;gd.input3(1,aCPC);
double aVPC324[]={9.4837,2397.26,-30.88,0.0};aVPC=aVPC324;gd.input4(3,aVPC);
gd.input5(162300.0,198600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName325[]={"C","H"};atomName=atomName325;double atomN325[]={4.0,6.0};atomN=atomN325;
gd.input1(325,"C4H6","1,3-butadiene",atomName,atomN);
gd.input2(54.092,164.2,268.7,425.0,43.3,221.0,0.27,0.195,0.0);
double aCPC325[]={-1.687,0.3419,-2.34E-4,6.335E-8};aCPC=aCPC325;gd.input3(1,aCPC);
double aVPC325[]={-7.12563,1.73913,-2.70805,-1.68376};aVPC=aVPC325;gd.input4(1,aVPC);
gd.input5(110200.0,150800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName326[]={"C","H","O"};atomName=atomName326;double atomN326[]={4.0,6.0,2.0};atomN=atomN326;
gd.input1(326,"C4H6O2","vinylacetate",atomName,atomN);
gd.input2(86.091,173.0,346.0,525.0,43.5,265.0,0.26,0.34,1.7);
double aCPC326[]={15.16,0.2795,-8.805E-5,-1.66E-8};aCPC=aCPC326;gd.input3(1,aCPC);
double aVPC326[]={-7.80478,1.80668,-4.4816,1.70357};aVPC=aVPC326;gd.input4(1,aVPC);
gd.input5(-316000.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName327[]={"C","H","O"};atomName=atomName327;double atomN327[]={4.0,6.0,3.0};atomN=atomN327;
gd.input1(327,"C4H6O3","aceticanhydride",atomName,atomN);
gd.input2(102.089,199.0,413.2,569.0,46.8,0.0,0.0,0.908,3.0);
double aCPC327[]={-23.13,0.5087,-3.58E-4,9.835E-8};aCPC=aCPC327;gd.input3(1,aCPC);
double aVPC327[]={18.1529,18.3036,20.0953,16.697};aVPC=aVPC327;gd.input4(1,aVPC);
gd.input5(-576100.0,-477000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName328[]={"C","H","O"};atomName=atomName328;double atomN328[]={4.0,6.0,4.0};atomN=atomN328;
gd.input1(328,"C4H6O4","dimethyloxalate",atomName,atomN);
gd.input2(118.09,327.0,436.5,628.0,39.8,0.0,0.0,0.556,0.0);
double aCPC328[]={0.0,0.0,0.0,0.0};aCPC=aCPC328;gd.input3(1,aCPC);
double aVPC328[]={0.0,0.0,0.0,0.0};aVPC=aVPC328;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName329[]={"C","H","O"};atomName=atomName329;double atomN329[]={4.0,6.0,4.0};atomN=atomN329;
gd.input1(329,"C4H6O4","succinicacid",atomName,atomN);
gd.input2(118.09,456.0,508.0,0.0,0.0,0.0,0.0,0.0,2.2);
double aCPC329[]={15.07,0.4689,-3.143E-4,7.938E-8};aCPC=aCPC329;gd.input3(1,aCPC);
double aVPC329[]={0.0,0.0,0.0,0.0};aVPC=aVPC329;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName330[]={"C","H","N"};atomName=atomName330;double atomN330[]={4.0,7.0,1.0};atomN=atomN330;
gd.input1(330,"C4H7N","butylonitrile",atomName,atomN);
gd.input2(69.107,161.0,391.1,582.2,37.9,0.0,0.0,0.373,3.8);
double aCPC330[]={15.21,0.3206,-1.638E-4,2.982E-8};aCPC=aCPC330;gd.input3(1,aCPC);
double aVPC330[]={49.985,6476.68,-5.599,3770.0};aVPC=aVPC330;gd.input4(2,aVPC);
gd.input5(34100.0,108700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName331[]={"C","H","O"};atomName=atomName331;double atomN331[]={4.0,7.0,2.0};atomN=atomN331;
gd.input1(331,"C4H7O2","methylacrylate",atomName,atomN);
gd.input2(86.091,196.7,353.5,536.0,43.0,265.0,0.25,0.35,0.0);
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double aCPC331[]={15.16,0.2796,-8.805E-5,-1.66E-8};aCPC=aCPC331;gd.input3(1,aCPC);
double aVPC331[]={9.4886,2788.43,-59.15,0.0};aVPC=aVPC331;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName332[]={"C","H"};atomName=atomName332;double atomN332[]={4.0,8.0};atomN=atomN332;
gd.input1(332,"C4H8","1-butene",atomName,atomN);
gd.input2(56.108,87.8,266.9,419.6,40.2,240.0,0.277,0.191,0.3);
double aCPC332[]={-2.994,0.3532,-1.99E-4,4.463E-8};aCPC=aCPC332;gd.input3(1,aCPC);
double aVPC332[]={-6.88204,1.27051,-2.26284,-2.61632};aVPC=aVPC332;gd.input4(1,aVPC);
gd.input5(-126.0,71340.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName333[]={"C","H"};atomName=atomName333;double atomN333[]={4.0,8.0};atomN=atomN333;
gd.input1(333,"C4H8","2-butene,cis",atomName,atomN);
gd.input2(56.108,134.3,276.9,435.6,42.0,234.0,0.271,0.202,0.3);
double aCPC333[]={0.4396,0.2953,-1.108E-4,-6.16E-10};aCPC=aCPC333;gd.input3(1,aCPC);
double aVPC333[]={-6.88706,1.15941,-2.19304,-3.12758};aVPC=aVPC333;gd.input4(1,aVPC);
gd.input5(-6990.0,-65900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName334[]={"C","H"};atomName=atomName334;double atomN334[]={4.0,8.0};atomN=atomN334;
gd.input1(334,"C4H8","2-butene,trans",atomName,atomN);
gd.input2(56.108,167.6,274.0,428.6,39.9,238.0,0.266,0.205,0.0);
double aCPC334[]={18.32,0.2564,-7.013E-5,-8.989E-9};aCPC=aCPC334;gd.input3(1,aCPC);
double aVPC334[]={43.517,4174.56,-5.041,1995.0};aVPC=aVPC334;gd.input4(2,aVPC);
gd.input5(-11180.0,63010.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName335[]={"C","H"};atomName=atomName335;double atomN335[]={4.0,8.0};atomN=atomN335;
gd.input1(335,"C4H8","cyclobutane",atomName,atomN);
gd.input2(56.108,182.4,285.7,460.0,49.9,210.0,0.274,0.181,0.0);
double aCPC335[]={-50.25,0.5024,-3.558E-4,1.047E-7};aCPC=aCPC335;gd.input3(1,aCPC);
double aVPC335[]={-7.40011,2.37997,-3.12269,-0.3431};aVPC=aVPC335;gd.input4(1,aVPC);
gd.input5(26670.0,110100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName336[]={"C","H"};atomName=atomName336;double atomN336[]={4.0,8.0};atomN=atomN336;
gd.input1(336,"C4H8","isobutylene",atomName,atomN);
gd.input2(56.108,132.8,266.2,417.9,40.0,239.0,0.275,0.194,0.5);
double aCPC336[]={16.05,0.2804,-1.091E-4,9.098E-9};aCPC=aCPC336;gd.input3(1,aCPC);
double aVPC336[]={-6.95542,1.35673,-2.45222,-1.4611};aVPC=aVPC336;gd.input4(1,aVPC);
gd.input5(-16910.0,58110.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName337[]={"C","H","O"};atomName=atomName337;double atomN337[]={4.0,8.0,1.0};atomN=atomN337;
gd.input1(337,"C4H8O","n-butyraldehyde",atomName,atomN);
gd.input2(72.107,176.8,348.0,545.4,53.8,0.0,0.0,0.352,2.6);
double aCPC337[]={14.08,0.3457,-1.743E-4,2.887E-8};aCPC=aCPC337;gd.input3(1,aCPC);
double aVPC337[]={-7.01403,0.12265,-7.3E-4,-8.50911};aVPC=aVPC337;gd.input4(1,aVPC);
gd.input5(-205200.0,-114800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName338[]={"C","H","O"};atomName=atomName338;double atomN338[]={4.0,8.0,1.0};atomN=atomN338;
gd.input1(338,"C4H8O","isobutyraldehyde",atomName,atomN);
gd.input2(72.107,208.2,337.0,513.0,41.5,274.0,0.27,0.35,0.0);
double aCPC338[]={24.46,0.3356,-2.057E-4,6.368E-8};aCPC=aCPC338;gd.input3(1,aCPC);
double aVPC338[]={-7.53679,1.08548,-1.52929,-8.48589};aVPC=aVPC338;gd.input4(1,aVPC);
gd.input5(-215900.0,-121400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName339[]={"C","H","O"};atomName=atomName339;double atomN339[]={4.0,8.0,1.0};atomN=atomN339;
gd.input1(339,"C4H8O","methylethylketone",atomName,atomN);
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gd.input2(72.107,186.5,352.7,536.8,42.1,267.0,0.252,0.32,3.3);
double aCPC339[]={10.94,0.3559,-1.9E-4,3.92E-8};aCPC=aCPC339;gd.input3(1,aCPC);
double aVPC339[]={-7.71476,1.71061,-3.6877,-0.75169};aVPC=aVPC339;gd.input4(1,aVPC);
gd.input5(-238500.0,-146200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName340[]={"C","H","O"};atomName=atomName340;double atomN340[]={4.0,8.0,1.0};atomN=atomN340;
gd.input1(340,"C4H8O","tetrahydrofuran",atomName,atomN);
gd.input2(72.107,164.7,338.0,540.1,51.9,224.0,0.259,0.217,1.7);
double aCPC340[]={19.1,0.5162,-4.132E-4,1.454E-7};aCPC=aCPC340;gd.input3(1,aCPC);
double aVPC340[]={9.4867,2768.38,-46.9,0.0};aVPC=aVPC340;gd.input4(3,aVPC);
gd.input5(-184300.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName341[]={"C","H","O"};atomName=atomName341;double atomN341[]={4.0,8.0,1.0};atomN=atomN341;
gd.input1(341,"C4H8O","vinylethylether",atomName,atomN);
gd.input2(72.107,157.9,308.7,475.0,40.7,0.0,0.0,0.268,1.3);
double aCPC341[]={17.28,0.3236,-1.471E-4,2.15E-8};aCPC=aCPC341;gd.input3(1,aCPC);
double aVPC341[]={-7.33727,1.50878,-3.30376,-1.10728};aVPC=aVPC341;gd.input4(1,aVPC);
gd.input5(-140300.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName342[]={"C","H","O"};atomName=atomName342;double atomN342[]={4.0,8.0,2.0};atomN=atomN342;
gd.input1(342,"C4H8O2","n-butyricacid",atomName,atomN);
gd.input2(88.107,267.9,437.2,628.0,52.7,290.0,0.292,0.683,1.5);
double aCPC342[]={11.74,0.4137,-2.43E-4,5.531E-8};aCPC=aCPC342;gd.input3(1,aCPC);
double aVPC342[]={-10.0392,3.15679,-7.72604,5.2763};aVPC=aVPC342;gd.input4(1,aVPC);
gd.input5(-476200.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName343[]={"C","H","O"};atomName=atomName343;double atomN343[]={4.0,8.0,2.0};atomN=atomN343;
gd.input1(343,"C4H8O2","isobutyricacid",atomName,atomN);
gd.input2(88.107,227.2,427.9,609.0,40.5,292.0,0.234,0.623,1.3);
double aCPC343[]={9.814,0.4668,-3.72E-4,1.35E-7};aCPC=aCPC343;gd.input3(1,aCPC);
double aVPC343[]={76.037,9222.72,-8.986,3863.0};aVPC=aVPC343;gd.input4(2,aVPC);
gd.input5(-484200.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName344[]={"C","H","O"};atomName=atomName344;double atomN344[]={4.0,8.0,2.0};atomN=atomN344;
gd.input1(344,"C4H8O2","1,4-dioxane",atomName,atomN);
gd.input2(88.107,285.0,374.6,587.0,52.1,238.0,0.254,0.281,0.4);
double aCPC344[]={-53.57,0.5987,-4.085E-4,1.062E-7};aCPC=aCPC344;gd.input3(1,aCPC);
double aVPC344[]={9.5125,2966.88,-62.15,0.0};aVPC=aVPC344;gd.input4(3,aVPC);
gd.input5(-315300.0,-180900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName345[]={"C","H","O"};atomName=atomName345;double atomN345[]={4.0,8.0,2.0};atomN=atomN345;
gd.input1(345,"C4H8O2","ethylacetate",atomName,atomN);
gd.input2(88.107,189.6,350.3,523.2,38.3,286.0,0.252,0.362,1.9);
double aCPC345[]={7.235,0.4072,-2.092E-4,2.855E-8};aCPC=aCPC345;gd.input3(1,aCPC);
double aVPC345[]={-7.68521,1.36511,-4.0898,-1.75342};aVPC=aVPC345;gd.input4(1,aVPC);
gd.input5(-443200.0,-327600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName346[]={"C","H","O"};atomName=atomName346;double atomN346[]={4.0,8.0,2.0};atomN=atomN346;
gd.input1(346,"C4H8O2","methylpropionate",atomName,atomN);
gd.input2(88.107,185.7,352.8,530.6,40.0,282.0,0.256,0.35,1.7);
double aCPC346[]={18.2,0.314,-9.353E-5,-1.828E-8};aCPC=aCPC346;gd.input3(1,aCPC);
double aVPC346[]={-8.23756,2.71406,-5.35097,-2.34114};aVPC=aVPC346;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName347[]={"C","H","O"};atomName=atomName347;double atomN347[]={4.0,8.0,2.0};atomN=atomN347;
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gd.input1(347,"C4H8O2","n-propylformate",atomName,atomN);
gd.input2(88.107,180.3,354.1,538.0,40.6,285.0,0.259,0.314,1.9);
double aCPC347[]={0.0,0.0,0.0,0.0};aCPC=aCPC347;gd.input3(1,aCPC);
double aVPC347[]={-7.48563,1.7126,-5.16404,1.6429};aVPC=aVPC347;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName348[]={"C","H","S"};atomName=atomName348;double atomN348[]={4.0,8.0,1.0};atomN=atomN348;
gd.input1(348,"C4H8S","tetrahydrothiophene",atomName,atomN);
gd.input2(88.172,177.0,394.2,632.0,0.0,0.0,0.0,0.0,1.9);
double aCPC348[]={0.0,0.0,0.0,0.0};aCPC=aCPC348;gd.input3(1,aCPC);
double aVPC348[]={9.387,3160.1,-57.2,0.0};aVPC=aVPC348;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName349[]={"C","H","Cl"};atomName=atomName349;double atomN349[]={4.0,9.0,1.0};atomN=atomN349;
gd.input1(349,"C4H9Cl","1-chlorobutane",atomName,atomN);
gd.input2(92.569,150.1,351.6,542.0,36.8,312.0,0.255,0.218,2.0);
double aCPC349[]={-2.613,0.4497,-2.937E-4,8.018E-8};aCPC=aCPC349;gd.input3(1,aCPC);
double aVPC349[]={-6.79852,0.78511,-2.31047,-5.83223};aVPC=aVPC349;gd.input4(1,aVPC);
gd.input5(-147400.0,-38810.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName350[]={"C","H","Cl"};atomName=atomName350;double atomN350[]={4.0,9.0,1.0};atomN=atomN350;
gd.input1(350,"C4H9Cl","2-chlorobutane",atomName,atomN);
gd.input2(92.569,141.8,341.4,520.6,39.5,305.0,0.28,0.3,2.1);
double aCPC350[]={-3.433,0.4559,-2.981E-4,8.256E-8};aCPC=aCPC350;gd.input3(1,aCPC);
double aVPC350[]={9.3705,2753.43,-47.15,0.0};aVPC=aVPC350;gd.input4(3,aVPC);
gd.input5(-161600.0,-53510.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName351[]={"C","H","Cl"};atomName=atomName351;double atomN351[]={4.0,9.0,1.0};atomN=atomN351;
gd.input1(351,"C4H9Cl","tert-butylchloride",atomName,atomN);
gd.input2(92.569,247.8,324.0,507.0,39.5,295.0,0.28,0.19,2.1);
double aCPC351[]={-3.931,0.4652,-2.886E-4,7.871E-8};aCPC=aCPC351;gd.input3(1,aCPC);
double aVPC351[]={9.1919,2567.15,-44.15,0.0};aVPC=aVPC351;gd.input4(3,aVPC);
gd.input5(-183400.0,-64140.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName352[]={"C","H","N"};atomName=atomName352;double atomN352[]={4.0,9.0,1.0};atomN=atomN352;
gd.input1(352,"C4H9N","pyrrolidine",atomName,atomN);
gd.input2(71.123,0.0,359.6,568.6,56.1,249.0,0.295,0.274,1.6);
double aCPC352[]={-51.53,0.5338,-3.24E-4,7.528E-8};aCPC=aCPC352;gd.input3(1,aCPC);
double aVPC352[]={-7.73658,2.33495,-4.20213,-3.71251};aVPC=aVPC352;gd.input4(1,aVPC);
gd.input5(-3600.0,114800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName353[]={"C","H"};atomName=atomName353;double atomN353[]={4.0,10.0};atomN=atomN353;
gd.input1(353,"C4H10","isobutane",atomName,atomN);
gd.input2(58.124,113.6,261.4,408.2,36.5,263.0,0.283,0.183,0.1);
double aCPC353[]={-1.39,0.3847,-1.846E-4,2.895E-8};aCPC=aCPC353;gd.input3(1,aCPC);
double aVPC353[]={-6.95579,1.5009,-2.52717,-1.49776};aVPC=aVPC353;gd.input4(1,aVPC);
gd.input5(-134600.0,-20900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName354[]={"C","H","O"};atomName=atomName354;double atomN354[]={4.0,10.0,1.0};atomN=atomN354;
gd.input1(354,"C4H10O","n-butanol",atomName,atomN);
gd.input2(74.123,183.9,390.9,563.1,44.2,275.0,0.259,0.593,1.8);
double aCPC354[]={3.266,0.418,-2.242E-4,4.685E-8};aCPC=aCPC354;gd.input3(1,aCPC);
double aVPC354[]={-8.00756,0.53783,-9.3424,6.68692};aVPC=aVPC354;gd.input4(1,aVPC);
gd.input5(-274900.0,-150900.0);
gi.addElement(gd);

gd=new Gas_Data();
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String atomName355[]={"C","H","O"};atomName=atomName355;double atomN355[]={4.0,10.0,1.0};atomN=atomN355;
gd.input1(355,"C4H10O","2-butanol",atomName,atomN);
gd.input2(74.123,158.5,372.7,536.1,41.8,269.0,0.252,0.577,1.7);
double aCPC355[]={5.753,0.4245,-2.328E-4,4.773E-8};aCPC=aCPC355;gd.input3(1,aCPC);
double aVPC355[]={-7.80578,0.32456,-9.41265,2.64643};aVPC=aVPC355;gd.input4(1,aVPC);
gd.input5(-292800.0,-167700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName356[]={"C","H","O"};atomName=atomName356;double atomN356[]={4.0,10.0,1.0};atomN=atomN356;
gd.input1(356,"C4H10O","isobutanol",atomName,atomN);
gd.input2(74.123,165.2,381.0,547.8,43.0,273.0,0.257,0.592,1.7);
double aCPC356[]={-7.708,0.4689,-2.884E-4,7.231E-8};aCPC=aCPC356;gd.input3(1,aCPC);
double aVPC356[]={10.251,2874.73,-100.3,0.0};aVPC=aVPC356;gd.input4(3,aVPC);
gd.input5(-283400.0,-167400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName357[]={"C","H","O"};atomName=atomName357;double atomN357[]={4.0,10.0,1.0};atomN=atomN357;
gd.input1(357,"C4H10O","tert-butanol",atomName,atomN);
gd.input2(74.123,298.8,355.5,506.2,39.7,275.0,0.259,0.612,1.7);
double aCPC357[]={-46.81,0.7172,-7.084E-4,2.92E-7};aCPC=aCPC357;gd.input3(1,aCPC);
double aVPC357[]={10.2436,2658.29,-90.5,0.0};aVPC=aVPC357;gd.input4(3,aVPC);
gd.input5(-312800.0,-177800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName358[]={"C","H","O"};atomName=atomName358;double atomN358[]={4.0,10.0,1.0};atomN=atomN358;
gd.input1(358,"C4H10O","diethylether",atomName,atomN);
gd.input2(74.123,156.9,307.6,466.7,36.4,280.0,0.262,0.281,1.3);
double aCPC358[]={21.42,0.3359,-1.035E-4,-9.357E-9};aCPC=aCPC358;gd.input3(1,aCPC);
double aVPC358[]={-7.29916,1.24828,-2.91931,-3.3674};aVPC=aVPC358;gd.input4(1,aVPC);
gd.input5(-252400.0,-122400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName359[]={"C","H","O"};atomName=atomName359;double atomN359[]={4.0,10.0,1.0};atomN=atomN359;
gd.input1(359,"C4H10O","methylpropylether",atomName,atomN);
gd.input2(74.123,0.0,311.7,476.3,38.0,0.0,0.0,0.271,1.2);
double aCPC359[]={21.31,0.339,-1.127E-4,-2.855E-9};aCPC=aCPC359;gd.input3(1,aCPC);
double aVPC359[]={-7.5983,2.01601,-3.7039,-1.6471};aVPC=aVPC359;gd.input4(1,aVPC);
gd.input5(-237900.0,-110000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName360[]={"C","H","O"};atomName=atomName360;double atomN360[]={4.0,10.0,1.0};atomN=atomN360;
gd.input1(360,"C4H10O","methylisopropylether",atomName,atomN);
gd.input2(74.123,0.0,303.9,464.5,37.6,0.0,0.0,0.266,0.0);
double aCPC360[]={13.53,0.3697,-1.481E-4,1.205E-8};aCPC=aCPC360;gd.input3(1,aCPC);
double aVPC360[]={-7.06696,0.86497,-2.16269,-4.72211};aVPC=aVPC360;gd.input4(1,aVPC);
gd.input5(-252200.0,-121000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName361[]={"C","H","O"};atomName=atomName361;double atomN361[]={4.0,10.0,2.0};atomN=atomN361;
gd.input1(361,"C4H10O2","1,2-dimethoxyethane",atomName,atomN);
gd.input2(90.123,202.0,358.0,536.0,38.7,271.0,0.235,0.358,0.0);
double aCPC361[]={32.23,0.3567,-1.336E-4,8.399E-9};aCPC=aCPC361;gd.input3(1,aCPC);
double aVPC361[]={9.4039,2869.79,-53.15,0.0};aVPC=aVPC361;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName362[]={"C","H","O"};atomName=atomName362;double atomN362[]={4.0,10.0,3.0};atomN=atomN362;
gd.input1(362,"C4H10O3","diethyleneglycol",atomName,atomN);
gd.input2(106.122,265.0,519.0,681.0,47.0,0.0,0.0,0.0,0.0);
double aCPC362[]={73.06,0.3461,-1.468E-4,1.846E-8};aCPC=aCPC362;gd.input3(1,aCPC);
double aVPC362[]={10.4124,4122.52,-122.5,0.0};aVPC=aVPC362;gd.input4(3,aVPC);
gd.input5(-571500.0,0.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName363[]={"C","H","S"};atomName=atomName363;double atomN363[]={4.0,10.0,1.0};atomN=atomN363;
gd.input1(363,"C4H10S","diethylsulfide",atomName,atomN);
gd.input2(90.184,169.2,365.3,557.0,39.6,318.0,0.272,0.292,1.6);
double aCPC363[]={13.59,0.3959,-1.78E-4,2.649E-8};aCPC=aCPC363;gd.input3(1,aCPC);
double aVPC363[]={9.3329,2896.27,-54.49,0.0};aVPC=aVPC363;gd.input4(3,aVPC);
gd.input5(-83530.0,17800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName364[]={"C","H","S"};atomName=atomName364;double atomN364[]={4.0,10.0,2.0};atomN=atomN364;
gd.input1(364,"C4H10S2","diethyldisulfide",atomName,atomN);
gd.input2(122.244,171.7,427.1,642.0,0.0,0.0,0.0,0.0,2.0);
double aCPC364[]={26.9,0.4601,-2.71E-4,5.97E-8};aCPC=aCPC364;gd.input3(1,aCPC);
double aVPC364[]={9.4405,3421.57,-64.19,0.0};aVPC=aVPC364;gd.input4(3,aVPC);
gd.input5(-74690.0,22270.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName365[]={"C","H","N"};atomName=atomName365;double atomN365[]={4.0,11.0,1.0};atomN=atomN365;
gd.input1(365,"C4H11N","n-butylamine",atomName,atomN);
gd.input2(73.139,224.1,349.5,531.9,42.0,0.0,0.0,0.329,1.3);
double aCPC365[]={5.079,0.4476,-2.407E-4,7.599E-8};aCPC=aCPC365;gd.input3(1,aCPC);
double aVPC365[]={-7.91668,2.36401,-5.0117,-2.54215};aVPC=aVPC365;gd.input4(1,aVPC);
gd.input5(-92110.0,49240.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName366[]={"C","H","N"};atomName=atomName366;double atomN366[]={4.0,11.0,1.0};atomN=atomN366;
gd.input1(366,"C4H11N","isobutylamine",atomName,atomN);
gd.input2(73.139,188.0,336.2,514.3,41.0,0.0,0.0,0.368,1.2);
double aCPC366[]={9.491,0.443,-2.11E-4,2.333E-8};aCPC=aCPC366;gd.input3(1,aCPC);
double aVPC366[]={-8.41366,3.12108,-5.70064,-1.8392};aVPC=aVPC366;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName367[]={"C","H","N"};atomName=atomName367;double atomN367[]={4.0,11.0,1.0};atomN=atomN367;
gd.input1(367,"C4H11N","diethylamine",atomName,atomN);
gd.input2(73.139,223.4,328.6,496.5,37.1,301.0,0.271,0.291,1.1);
double aCPC367[]={2.039,0.443,-2.183E-4,3.653E-8};aCPC=aCPC367;gd.input3(1,aCPC);
double aVPC367[]={-7.26796,1.1581,-3.91125,-1.17981};aVPC=aVPC367;gd.input4(1,aVPC);
gd.input5(-72430.0,72140.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName368[]={"C","H"};atomName=atomName368;double atomN368[]={5.0,12.0};atomN=atomN368;
gd.input1(368,"C5F12","perfluoropentane",atomName,atomN);
gd.input2(288.031,0.0,302.4,420.6,20.5,473.0,0.276,0.432,0.0);
double aCPC368[]={0.0,0.0,0.0,0.0};aCPC=aCPC368;gd.input3(1,aCPC);
double aVPC368[]={9.539,2470.33,-43.2,0.0};aVPC=aVPC368;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName369[]={"C","H","F","O"};atomName=atomName369;double atomN369[]={5.0,2.0,6.0,2.0};atomN=atomN369;
gd.input1(369,"C5H2F6O2","hexafluoroacetylacetone",atomName,atomN);
gd.input2(208.059,0.0,327.3,485.1,27.7,0.0,0.0,0.278,0.0);
double aCPC369[]={0.0,0.0,0.0,0.0};aCPC=aCPC369;gd.input3(1,aCPC);
double aVPC369[]={0.0,0.0,0.0,0.0};aVPC=aVPC369;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName370[]={"C","H","O"};atomName=atomName370;double atomN370[]={5.0,4.0,2.0};atomN=atomN370;
gd.input1(370,"C5H4O2","furfural",atomName,atomN);
gd.input2(96.085,234.5,434.9,670.0,58.9,0.0,0.0,0.383,3.6);
double aCPC370[]={0.0,0.0,0.0,0.0};aCPC=aCPC370;gd.input3(1,aCPC);
double aVPC370[]={8.5214,2760.09,-110.4,0.0};aVPC=aVPC370;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);
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gd=new Gas_Data();
String atomName371[]={"C","H","N"};atomName=atomName371;double atomN371[]={5.0,5.0,1.0};atomN=atomN371;
gd.input1(371,"C5H5N","pyridine",atomName,atomN);
gd.input2(79.102,231.5,388.4,620.0,56.3,254.0,0.277,0.243,2.3);
double aCPC371[]={39.79,0.4928,-3.558E-4,1.004E-7};aCPC=aCPC371;gd.input3(1,aCPC);
double aVPC371[]={-7.07689,1.21511,-2.76681,-2.87472};aVPC=aVPC371;gd.input4(1,aVPC);
gd.input5(1.403E-5,190300.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName372[]={"C","H","N"};atomName=atomName372;double atomN372[]={5.0,6.0,2.0};atomN=atomN372;
gd.input1(372,"C5H6N2","2-methylpyrazine",atomName,atomN);
gd.input2(94.117,0.0,410.0,634.3,50.1,283.0,0.268,0.315,0.0);
double aCPC372[]={0.0,0.0,0.0,0.0};aCPC=aCPC372;gd.input3(1,aCPC);
double aVPC372[]={0.0,0.0,0.0,0.0};aVPC=aVPC372;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName373[]={"C","H","O"};atomName=atomName373;double atomN373[]={5.0,6.0,1.0};atomN=atomN373;
gd.input1(373,"C5H6O","2-methylfuran",atomName,atomN);
gd.input2(82.102,0.0,338.0,527.0,47.2,247.0,0.266,0.27,0.7);
double aCPC373[]={0.0,0.0,0.0,0.0};aCPC=aCPC373;gd.input3(1,aCPC);
double aVPC373[]={0.0,0.0,0.0,0.0};aVPC=aVPC373;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName374[]={"C","H"};atomName=atomName374;double atomN374[]={5.0,8.0};atomN=atomN374;
gd.input1(374,"C5H8","cyclopentene",atomName,atomN);
gd.input2(68.119,138.1,317.4,506.0,0.0,0.0,0.0,0.0,0.9);
double aCPC374[]={-41.51,0.4631,-2.579E-4,5.434E-8};aCPC=aCPC374;gd.input3(1,aCPC);
double aVPC374[]={9.3154,2583.07,-39.7,0.0};aVPC=aVPC374;gd.input4(3,aVPC);
gd.input5(32950.0,110900.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName375[]={"C","H"};atomName=atomName375;double atomN375[]={5.0,8.0};atomN=atomN375;
gd.input1(375,"C5H8","1,2-pentadiene",atomName,atomN);
gd.input2(68.119,135.9,318.0,503.0,40.7,276.0,0.269,0.173,0.0);
double aCPC375[]={8.826,0.388,-2.28E-4,5.246E-8};aCPC=aCPC375;gd.input3(1,aCPC);
double aVPC375[]={9.3095,2544.34,-44.3,0.0};aVPC=aVPC375;gd.input4(3,aVPC);
gd.input5(145700.0,210600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName376[]={"C","H"};atomName=atomName376;double atomN376[]={5.0,8.0};atomN=atomN376;
gd.input1(376,"C5H8","1,3-pentadiene,trans",atomName,atomN);
gd.input2(68.119,185.7,315.1,496.0,39.9,275.0,0.266,0.175,0.7);
double aCPC376[]={30.69,0.2811,-6.711E-5,-2.352E-8};aCPC=aCPC376;gd.input3(1,aCPC);
double aVPC376[]={9.298,2541.69,-41.43,0.0};aVPC=aVPC376;gd.input4(3,aVPC);
gd.input5(77870.0,146800.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName377[]={"C","H"};atomName=atomName377;double atomN377[]={5.0,8.0};atomN=atomN377;
gd.input1(377,"C5H8","1,4-pentadiene",atomName,atomN);
gd.input2(68.119,124.9,299.1,478.0,37.9,276.0,0.263,0.104,0.4);
double aCPC377[]={6.996,0.3952,-2.374E-4,5.598E-8};aCPC=aCPC377;gd.input3(1,aCPC);
double aVPC377[]={9.119,2344.02,-41.69,0.0};aVPC=aVPC377;gd.input4(3,aVPC);
gd.input5(105500.0,170400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName378[]={"C","H"};atomName=atomName378;double atomN378[]={5.0,8.0};atomN=atomN378;
gd.input1(378,"C5H8","pentyne",atomName,atomN);
gd.input2(68.119,167.5,313.3,493.5,40.5,278.0,0.275,0.164,0.9);
double aCPC378[]={18.07,0.3511,-1.913E-4,4.098E-8};aCPC=aCPC378;gd.input3(1,aCPC);
double aVPC378[]={9.4227,2515.52,-45.97,0.0};aVPC=aVPC378;gd.input4(3,aVPC);
gd.input5(144400.0,210400.0);
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gi.addElement(gd);

gd=new Gas_Data();
String atomName379[]={"C","H"};atomName=atomName379;double atomN379[]={5.0,8.0};atomN=atomN379;
gd.input1(379,"C5H8","2-methyl-1,3-butadiene",atomName,atomN);
gd.input2(68.119,127.2,307.2,484.0,38.5,276.0,0.264,0.164,0.3);
double aCPC379[]={-3.412,0.4585,-3.337E-4,1.0E-7};aCPC=aCPC379;gd.input3(1,aCPC);
double aVPC379[]={-6.59262,1.2893,-3.89168,1.70215};aVPC=aVPC379;gd.input4(1,aVPC);
gd.input5(75780.0,146000.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName380[]={"C","H"};atomName=atomName380;double atomN380[]={5.0,8.0};atomN=atomN380;
gd.input1(380,"C5H8","3-methyl-1,2-butadiene",atomName,atomN);
gd.input2(68.119,159.5,314.0,496.0,41.1,267.0,0.266,0.16,0.0);
double aCPC380[]={14.69,0.3598,-1.976E-4,4.262E-8};aCPC=aCPC380;gd.input3(1,aCPC);
double aVPC380[]={-6.71441,1.53531,-4.64262,2.99854};aVPC=aVPC380;gd.input4(1,aVPC);
gd.input5(129800.0,198700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName381[]={"C","H","O"};atomName=atomName381;double atomN381[]={5.0,8.0,1.0};atomN=atomN381;
gd.input1(381,"C5H8O","cyclopentanone",atomName,atomN);
gd.input2(84.118,222.5,403.9,634.6,51.1,268.0,0.26,0.35,3.0);
double aCPC381[]={-40.64,0.5255,-3.124E-4,7.13E-8};aCPC=aCPC381;gd.input3(1,aCPC);
double aVPC381[]={-7.19551,1.16379,-2.52546,-3.28861};aVPC=aVPC381;gd.input4(1,aVPC);
gd.input5(-192800.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName382[]={"C","H","O"};atomName=atomName382;double atomN382[]={5.0,8.0,1.0};atomN=atomN382;
gd.input1(382,"C5H8O","dihydropyran",atomName,atomN);
gd.input2(84.118,0.0,359.0,561.7,45.6,268.0,0.262,0.247,1.4);
double aCPC382[]={0.0,0.0,0.0,0.0};aCPC=aCPC382;gd.input3(1,aCPC);
double aVPC382[]={0.0,0.0,0.0,0.0};aVPC=aVPC382;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName383[]={"C","H","O"};atomName=atomName383;double atomN383[]={5.0,8.0,2.0};atomN=atomN383;
gd.input1(383,"C5H8O2","ethylacrylate",atomName,atomN);
gd.input2(100.118,201.0,373.0,552.0,37.4,320.0,0.261,0.4,0.0);
double aCPC383[]={16.81,3.69,-1.382E-4,-5.732E-9};aCPC=aCPC383;gd.input3(1,aCPC);
double aVPC383[]={9.4688,2974.94,-58.15,0.0};aVPC=aVPC383;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName384[]={"C","H"};atomName=atomName384;double atomN384[]={5.0,10.0};atomN=atomN384;
gd.input1(384,"C5H10","cyclopentane",atomName,atomN);
gd.input2(70.135,179.3,322.4,511.7,45.1,260.0,0.275,0.196,0.0);
double aCPC384[]={-53.62,0.5426,-3.031E-4,6.485E-8};aCPC=aCPC384;gd.input3(1,aCPC);
double aVPC384[]={-6.51809,0.38442,-1.11706,-4.50275};aVPC=aVPC384;gd.input4(1,aVPC);
gd.input5(-77290.0,38600.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName385[]={"C","H"};atomName=atomName385;double atomN385[]={5.0,10.0};atomN=atomN385;
gd.input1(385,"C5H10","1-pentene",atomName,atomN);
gd.input2(70.135,107.9,303.1,464.8,35.3,300.0,0.31,0.233,0.4);
double aCPC385[]={-0.134,0.4329,-2.317E-4,4.681E-8};aCPC=aCPC385;gd.input3(1,aCPC);
double aVPC385[]={-7.04875,1.17813,-2.45105,-2.21727};aVPC=aVPC385;gd.input4(1,aVPC);
gd.input5(-20930.0,79170.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName386[]={"C","H"};atomName=atomName386;double atomN386[]={5.0,10.0};atomN=atomN386;
gd.input1(386,"C5H10","2-pentene,cis",atomName,atomN);
gd.input2(70.135,121.7,310.1,476.0,36.5,0.0,0.0,0.251,0.0);
double aCPC386[]={-14.29,0.4601,-2.541E-4,5.455E-8};aCPC=aCPC386;gd.input3(1,aCPC);
double aVPC386[]={-6.8016,0.54458,-1.55279,-5.68029};aVPC=aVPC386;gd.input4(1,aVPC);
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gd.input5(-28090.0,71890.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName387[]={"C","H"};atomName=atomName387;double atomN387[]={5.0,10.0};atomN=atomN387;
gd.input1(387,"C5H10","2-pentene,trans",atomName,atomN);
gd.input2(70.135,132.9,309.5,475.0,36.6,0.0,0.0,0.259,0.0);
double aCPC387[]={1.947,0.4182,-2.178E-4,4.405E-8};aCPC=aCPC387;gd.input3(1,aCPC);
double aVPC387[]={-6.99461,1.00724,-2.42146,-2.51692};aVPC=aVPC387;gd.input4(1,aVPC);
gd.input5(-31780.0,69960.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName388[]={"C","H"};atomName=atomName388;double atomN388[]={5.0,10.0};atomN=atomN388;
gd.input1(388,"C5H10","2-methyl-1-butene",atomName,atomN);
gd.input2(70.135,135.6,304.3,465.0,34.5,0.0,0.0,0.236,0.5);
double aCPC388[]={10.57,0.3997,-1.946E-4,3.314E-8};aCPC=aCPC388;gd.input3(1,aCPC);
double aVPC388[]={-6.8299,0.7266,-2.15363,-3.62225};aVPC=aVPC388;gd.input4(1,aVPC);
gd.input5(-36340.0,65650.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName389[]={"C","H"};atomName=atomName389;double atomN389[]={5.0,10.0};atomN=atomN389;
gd.input1(389,"C5H10","2-methyl-2-butene",atomName,atomN);
gd.input2(70.135,139.3,311.7,470.0,34.5,0.0,0.0,0.244,0.0);
double aCPC389[]={11.8,0.3509,-1.117E-4,-5.807E-9};aCPC=aCPC389;gd.input3(1,aCPC);
double aVPC389[]={-7.71438,1.95946,-3.1571,-2.22515};aVPC=aVPC389;gd.input4(1,aVPC);
gd.input5(-42580.0,59700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName390[]={"C","H"};atomName=atomName390;double atomN390[]={5.0,10.0};atomN=atomN390;
gd.input1(390,"C5H10","3-methyl-1-butene",atomName,atomN);
gd.input2(70.135,104.7,293.3,450.0,35.1,0.0,0.0,0.209,0.0);
double aCPC390[]={21.74,0.389,-2.007E-4,4.011E-8};aCPC=aCPC390;gd.input3(1,aCPC);
double aVPC390[]={-7.1887,1.42502,-2.27292,-2.04323};aVPC=aVPC390;gd.input4(1,aVPC);
gd.input5(-28970.0,74820.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName391[]={"C","H","O"};atomName=atomName391;double atomN391[]={5.0,10.0,1.0};atomN=atomN391;
gd.input1(391,"C5H10O","valeraldehyde",atomName,atomN);
gd.input2(86.134,182.0,376.0,554.0,35.4,333.0,0.26,0.4,2.6);
double aCPC391[]={14.24,0.4329,-2.107E-4,3.162E-8};aCPC=aCPC391;gd.input3(1,aCPC);
double aVPC391[]={9.5421,3030.2,-58.15,0.0};aVPC=aVPC391;gd.input4(3,aVPC);
gd.input5(-228000.0,-108400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName392[]={"C","H","O"};atomName=atomName392;double atomN392[]={5.0,10.0,1.0};atomN=atomN392;
gd.input1(392,"C5H10O","methyl-n-propyl-ketone",atomName,atomN);
gd.input2(86.134,196.0,375.4,561.1,36.9,301.0,0.238,0.346,2.5);
double aCPC392[]={1.147,0.4802,-2.818E-4,6.661E-8};aCPC=aCPC392;gd.input3(1,aCPC);
double aVPC392[]={9.3829,2934.87,-62.25,0.0};aVPC=aVPC392;gd.input4(3,aVPC);
gd.input5(-258800.0,-137200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName393[]={"C","H","O"};atomName=atomName393;double atomN393[]={5.0,10.0,1.0};atomN=atomN393;
gd.input1(393,"C5H10O","methyl",atomName,atomN);
gd.input2(86.134,181.0,367.5,553.4,38.5,310.0,0.259,0.331,2.8);
double aCPC393[]={-2.914,0.4991,-2.935E-4,6.665E-8};aCPC=aCPC393;gd.input3(1,aCPC);
double aVPC393[]={7.5577,1993.12,-103.2,0.0};aVPC=aVPC393;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName394[]={"C","H","O"};atomName=atomName394;double atomN394[]={5.0,10.0,1.0};atomN=atomN394;
gd.input1(394,"C5H10O","diethyl-ketone",atomName,atomN);
gd.input2(86.134,234.2,375.1,561.0,37.3,336.0,0.269,0.344,2.7);
double aCPC394[]={30.01,0.3939,-1.907E-4,3.398E-8};aCPC=aCPC394;gd.input3(1,aCPC);
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double aVPC394[]={-7.70542,1.44422,-3.60173,-2.88141};aVPC=aVPC394;gd.input4(1,aVPC);
gd.input5(-258800.0,-135400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName395[]={"C","H","O"};atomName=atomName395;double atomN395[]={5.0,10.0,1.0};atomN=atomN395;
gd.input1(395,"C5H10O","2-methyl-tetrahydrofuran",atomName,atomN);
gd.input2(86.134,0.0,351.0,537.0,37.6,267.0,0.225,0.264,0.0);
double aCPC395[]={0.0,0.0,0.0,0.0};aCPC=aCPC395;gd.input3(1,aCPC);
double aVPC395[]={0.0,0.0,0.0,0.0};aVPC=aVPC395;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName396[]={"C","H","O"};atomName=atomName396;double atomN396[]={5.0,10.0,1.0};atomN=atomN396;
gd.input1(396,"C5H10O","tetrahydropyran",atomName,atomN);
gd.input2(86.134,0.0,361.0,572.2,47.7,263.0,0.263,0.218,1.6);
double aCPC396[]={0.0,0.0,0.0,0.0};aCPC=aCPC396;gd.input3(1,aCPC);
double aVPC396[]={0.0,0.0,0.0,0.0};aVPC=aVPC396;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName397[]={"C","H","O"};atomName=atomName397;double atomN397[]={5.0,10.0,2.0};atomN=atomN397;
gd.input1(397,"C5H10O2","n-valeric-acid",atomName,atomN);
gd.input2(102.134,239.0,459.5,651.0,0.0,0.0,0.0,0.0,0.0);
double aCPC397[]={13.39,0.5033,-2.931E-4,6.619E-8};aCPC=aCPC397;gd.input3(1,aCPC);
double aVPC397[]={11.0104,4092.15,-86.55,0.0};aVPC=aVPC397;gd.input4(3,aVPC);
gd.input5(-490700.0,-357400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName398[]={"C","H","O"};atomName=atomName398;double atomN398[]={5.0,10.0,2.0};atomN=atomN398;
gd.input1(398,"C5H10O2","isovaleric-acid",atomName,atomN);
gd.input2(102.134,0.0,449.7,634.0,0.0,0.0,0.0,0.0,1.0);
double aCPC398[]={0.0,0.0,0.0,0.0};aCPC=aCPC398;gd.input3(1,aCPC);
double aVPC398[]={2.4671,588.09,-261.9,0.0};aVPC=aVPC398;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName399[]={"C","H","O"};atomName=atomName399;double atomN399[]={5.0,10.0,2.0};atomN=atomN399;
gd.input1(399,"C5H10O2","isobutyl-formate",atomName,atomN);
gd.input2(102.134,178.0,371.4,554.0,37.3,352.0,0.285,0.396,1.9);
double aCPC399[]={19.85,0.4034,-1.436E-4,-7.402E-9};aCPC=aCPC399;gd.input3(1,aCPC);
double aVPC399[]={-8.01454,2.05091,-4.38201,-2.85582};aVPC=aVPC399;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName400[]={"C","H","O"};atomName=atomName400;double atomN400[]={5.0,10.0,2.0};atomN=atomN400;
gd.input1(400,"C5H10O2","n-propyl-acetate",atomName,atomN);
gd.input2(102.134,178.0,374.7,549.4,33.3,345.0,0.252,0.391,1.8);
double aCPC400[]={15.42,0.4501,-1.686E-4,-1.439E-8};aCPC=aCPC400;gd.input3(1,aCPC);
double aVPC400[]={-7.85524,1.43936,-4.30187,-3.04832};aVPC=aVPC400;gd.input4(1,aVPC);
gd.input5(-466000.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName401[]={"C","H","O"};atomName=atomName401;double atomN401[]={5.0,10.0,2.0};atomN=atomN401;
gd.input1(401,"C5H10O2","ethyl-propionate",atomName,atomN);
gd.input2(102.134,199.3,372.2,546.0,33.6,345.0,0.256,0.391,1.8);
double aCPC401[]={19.85,0.4034,-1.437E-4,-7.394E-9};aCPC=aCPC401;gd.input3(1,aCPC);
double aVPC401[]={-8.55094,3.10067,-6.99241,3.45112};aVPC=aVPC401;gd.input4(1,aVPC);
gd.input5(-470200.0,-323700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName402[]={"C","H","O"};atomName=atomName402;double atomN402[]={5.0,10.0,2.0};atomN=atomN402;
gd.input1(402,"C5H10O2","methyl-butyrate",atomName,atomN);
gd.input2(102.134,188.4,375.9,554.4,34.8,340.0,0.257,0.38,1.7);
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double aCPC402[]={0.0,0.0,0.0,0.0};aCPC=aCPC402;gd.input3(1,aCPC);
double aVPC402[]={-7.776,1.32028,-3.93963,-3.53112};aVPC=aVPC402;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName403[]={"C","H","O"};atomName=atomName403;double atomN403[]={5.0,10.0,2.0};atomN=atomN403;
gd.input1(403,"C5H10O2","methyl-isobutyrate",atomName,atomN);
gd.input2(102.134,185.4,365.5,540.8,34.3,339.0,0.259,0.362,2.0);
double aCPC403[]={0.0,0.0,0.0,0.0};aCPC=aCPC403;gd.input3(1,aCPC);
double aVPC403[]={-7.65814,1.29248,-3.85632,-3.49858};aVPC=aVPC403;gd.input4(1,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName404[]={"C","H"};atomName=atomName404;double atomN404[]={5.0,12.0};atomN=atomN404;
gd.input1(404,"C5H12","n-pentane",atomName,atomN);
gd.input2(72.151,143.4,309.2,469.7,33.7,304.0,0.263,0.251,0.0);
double aCPC404[]={-3.626,0.4873,-2.58E-4,5.305E-8};aCPC=aCPC404;gd.input3(1,aCPC);
double aVPC404[]={-7.28936,1.53679,-3.08367,-1.02456};aVPC=aVPC404;gd.input4(1,aVPC);
gd.input5(-146500.0,-8370.0);
double agC5H12[][]={{-27.126813975187588,521.1992993524339,10.181275845750339,-220.51174178596935,200.0,575.0},
{86.14090234694802,282.5734706400868,-63.70346903313784,-80.9365119887851,575.0,950.0},
{173.26683904829534,172.0307802703151,-227.91599537506545,-40.93213124441803,950.0,1325.0},
{258.4406876777329,84.12079473536514,-467.34808637785693,-15.328853542295601,1325.0,1700.0},
{306.62342662655004,45.694129157102935,-693.2333649523431,-6.692280620508739,1700.0,2075.0},
{335.2260732954842,27.09122334595136,-894.4283273572914,-3.284760969799828,2075.0,2450.0},
{352.45377939585694,17.625065734544574,-1064.0060339762979,-1.8204393362400153,2450.0,2825.0},
{362.7972711563928,12.704444880672805,-1199.734279880342,-1.1615914763738098,2825.0,3200.0},
{369.24950190466745,10.00031566382144,-1308.7722149998974,-0.8426638933036465,3200.0,3575.0},
{374.17635623346683,8.158426040085725,-1413.3754781618277,-0.6489052471332123,3575.0,3950.0},
{379.7103590231169,6.29205717784193,-1557.7076208316132,-0.471804640403573,3950.0,4325.0},
{387.9500441887105,3.7569839864808676,-1815.8719561642276,-0.2523707566814986,4325.0,4700.0},
{401.04877085103715,0.04821246057329526,-2300.385748550535,0.04305071434074059,4700.0,5075.0},
{421.2971429502373,-5.2630855476351925,-3172.952811926648,0.4349780420651342,5075.0,5450.0},
{459.68496988483906,-14.573621205206207,-5108.1605692662315,1.0702720949371436,5450.0,6000.0}};
gd.inputCp(agC5H12);
gi.addElement(gd);

gd=new Gas_Data();
String atomName405[]={"C","H"};atomName=atomName405;double atomN405[]={5.0,12.0};atomN=atomN405;
gd.input1(405,"C5H12","2-methyl-butane",atomName,atomN);
gd.input2(72.151,113.3,301.0,460.4,33.9,306.0,0.267,0.227,0.1);
double aCPC405[]={-9.525,0.5066,-2.729E-4,5.723E-8};aCPC=aCPC405;gd.input3(1,aCPC);
double aVPC405[]={-7.12727,1.38996,-2.54302,-2.45657};aVPC=aVPC405;gd.input4(1,aVPC);
gd.input5(-154600.0,-14820.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName406[]={"C","H"};atomName=atomName406;double atomN406[]={5.0,12.0};atomN=atomN406;
gd.input1(406,"C5H12","2-2-dimethylpropane",atomName,atomN);
gd.input2(72.151,256.6,282.6,433.8,32.0,303.0,0.269,0.197,0.0);
double aCPC406[]={-16.59,0.5552,-3.306E-4,7.633E-8};aCPC=aCPC406;gd.input3(1,aCPC);
double aVPC406[]={-6.89153,1.25019,-2.28233,-4.74891};aVPC=aVPC406;gd.input4(1,aVPC);
gd.input5(-166100.0,-15240.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName407[]={"C","H","O"};atomName=atomName407;double atomN407[]={5.0,12.0,1.0};atomN=atomN407;
gd.input1(407,"C5H12O","1-pentanol",atomName,atomN);
gd.input2(88.15,195.0,411.1,588.2,39.1,326.0,0.26,0.579,1.7);
double aCPC407[]={3.869,0.5045,-2.639E-4,5.12E-8};aCPC=aCPC407;gd.input3(1,aCPC);
double aVPC407[]={-8.97725,2.99791,-12.9596,8.84205};aVPC=aVPC407;gd.input4(1,aVPC);
gd.input5(-298900.0,-146100.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName408[]={"C","H","O"};atomName=atomName408;double atomN408[]={5.0,12.0,1.0};atomN=atomN408;
gd.input1(408,"C5H12O","2-methyl-1-butanol",atomName,atomN);
gd.input2(88.15,203.0,401.9,571.0,33.4,0.0,0.0,0.0,0.0);
double aCPC408[]={-9.483,0.5677,-3.481E-4,8.637E-8};aCPC=aCPC408;gd.input3(1,aCPC);
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double aVPC408[]={-9.26305,3.86947,-15.3562,12.1464};aVPC=aVPC408;gd.input4(1,aVPC);
gd.input5(-302700.0,-165700.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName409[]={"C","H","O"};atomName=atomName409;double atomN409[]={5.0,12.0,1.0};atomN=atomN409;
gd.input1(409,"C5H12O","3-methyl-1-butanol",atomName,atomN);
gd.input2(88.15,156.0,405.2,579.4,0.0,0.0,0.0,0.0,1.8);
double aCPC409[]={-9.542,0.5681,-3.485E-4,8.65E-8};aCPC=aCPC409;gd.input3(1,aCPC);
double aVPC409[]={10.0925,3026.43,-104.1,0.0};aVPC=aVPC409;gd.input4(3,aVPC);
gd.input5(-302300.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName410[]={"C","H","O"};atomName=atomName410;double atomN410[]={5.0,12.0,1.0};atomN=atomN410;
gd.input1(410,"C5H12O","2-methyl-2butanol",atomName,atomN);
gd.input2(88.15,264.4,375.5,545.0,39.5,0.0,0.0,0.0,1.9);
double aCPC410[]={-12.09,0.6096,-4.204E-4,1.228E-7};aCPC=aCPC410;gd.input3(1,aCPC);
double aVPC410[]={-8.66602,3.46689,-14.175,10.9679};aVPC=aVPC410;gd.input4(1,aVPC);
gd.input5(-329900.0,-165400.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName411[]={"C","H","O"};atomName=atomName411;double atomN411[]={5.0,12.0,1.0};atomN=atomN411;
gd.input1(411,"C5H12O","2,2-dimethyl-1-propanol",atomName,atomN);
gd.input2(88.15,327.0,386.3,549.0,0.0,0.0,0.0,0.0,0.0);
double aCPC411[]={12.15,0.5397,-3.16E-4,7.122E-8};aCPC=aCPC411;gd.input3(1,aCPC);
double aVPC411[]={11.5134,3694.96,-65.0,0.0};aVPC=aVPC411;gd.input4(3,aVPC);
gd.input5(-293100.0,-125500.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName412[]={"C","H","N","O"};atomName=atomName412;double atomN412[]={4.0,9.0,1.0,1.0};atomN=atomN412;
gd.input1(412,"C4H9N0","morpholine",atomName,atomN);
gd.input2(87.122,268.4,401.4,618.0,54.7,253.0,0.27,0.37,1.5);
double aCPC412[]={-42.8,0.5388,-2.666E-4,4.199E-8};aCPC=aCPC412;gd.input3(1,aCPC);
double aVPC412[]={9.6162,3171.35,-71.15,0.0};aVPC=aVPC412;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName413[]={"Al","Br"};atomName=atomName413;double atomN413[]={1.0,3.0};atomN=atomN413;
gd.input1(413,"AlBr3","aliminiumtribromide",atomName,atomN);
gd.input2(266.694,370.7,528.0,763.0,28.9,310.0,0.41,0.399,5.0);
double aCPC413[]={64.94,0.06098,-7.306E-5,2.978E-8};aCPC=aCPC413;gd.input3(1,aCPC);
double aVPC413[]={0.0,0.0,0.0,0.0};aVPC=aVPC413;gd.input4(0,aVPC);
gd.input5(-423300.0,-452200.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName414[]={"C","H","O"};atomName=atomName414;double atomN414[]={6.0,10.0,1.0};atomN=atomN414;
gd.input1(414,"C6H10O","cyclohexanone",atomName,atomN);
gd.input2(98.145,242.0,428.8,629.0,39.0,0.0,0.0,0.0,3.1);
double aCPC414[]={-37.81,0.5539,-1.953E-4,-1.534E-8};aCPC=aCPC414;gd.input3(1,aCPC);
double aVPC414[]={0.0,0.0,0.0,0.0};aVPC=aVPC414;gd.input4(0,aVPC);
gd.input5(-230300.0,-90810.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName415[]={"C","H","O"};atomName=atomName415;double atomN415[]={6.0,12.0,1.0};atomN=atomN415;
gd.input1(415,"C6H12O","methylbutylketone",atomName,atomN);
gd.input2(100.16,216.0,400.7,587.0,33.2,0.0,0.0,0.392,0.0);
double aCPC415[]={0.0,0.0,0.0,0.0};aCPC=aCPC415;gd.input3(1,aCPC);
double aVPC415[]={0.0,0.0,0.0,0.0};aVPC=aVPC415;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName416[]={"C","H","O"};atomName=atomName416;double atomN416[]={6.0,12.0,2.0};atomN=atomN416;
gd.input1(416,"C6H12O2","isoamylformate",atomName,atomN);
gd.input2(116.16,0.0,396.7,578.0,0.0,0.0,0.0,0.0,0.0);
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double aCPC416[]={0.0,0.0,0.0,0.0};aCPC=aCPC416;gd.input3(1,aCPC);
double aVPC416[]={0.0,0.0,0.0,0.0};aVPC=aVPC416;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName417[]={"C","H","O"};atomName=atomName417;double atomN417[]={6.0,14.0,1.0};atomN=atomN417;
gd.input1(417,"C6H14O","2-hexanol",atomName,atomN);
gd.input2(102.177,0.0,411.0,586.2,0.0,0.0,0.0,0.0,0.0);
double aCPC417[]={0.0,0.0,0.0,0.0};aCPC=aCPC417;gd.input3(1,aCPC);
double aVPC417[]={10.0989,3158.53,-99.98,0.0};aVPC=aVPC417;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName418[]={"C","H","O"};atomName=atomName418;double atomN418[]={6.0,14.0,1.0};atomN=atomN418;
gd.input1(418,"C6H14O","methylamylether",atomName,atomN);
gd.input2(102.177,0.0,372.0,546.5,30.4,392.0,0.262,0.347,0.0);
double aCPC418[]={0.0,0.0,0.0,0.0};aCPC=aCPC418;gd.input3(1,aCPC);
double aVPC418[]={0.0,0.0,0.0,0.0};aVPC=aVPC418;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName419[]={"C","F"};atomName=atomName419;double atomN419[]={7.0,8.0};atomN=atomN419;
gd.input1(419,"C7F8","perfluorotoluene",atomName,atomN);
gd.input2(236.061,0.0,377.7,534.5,27.1,428.0,0.26,0.475,0.0);
double aCPC419[]={0.0,0.0,0.0,0.0};aCPC=aCPC419;gd.input3(1,aCPC);
double aVPC419[]={0.0,0.0,0.0,0.0};aVPC=aVPC419;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName420[]={"C","H","N"};atomName=atomName420;double atomN420[]={7.0,9.0,1.0};atomN=atomN420;
gd.input1(420,"C7H9N","2,3-dimethylpyridine",atomName,atomN);
gd.input2(107.156,0.0,434.4,655.4,0.0,0.0,0.0,0.0,2.2);
double aCPC420[]={0.0,0.0,0.0,0.0};aCPC=aCPC420;gd.input3(1,aCPC);
double aVPC420[]={10.529,4219.74,-33.04,0.0};aVPC=aVPC420;gd.input4(3,aVPC);
gd.input5(68290.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName421[]={"C","H","N"};atomName=atomName421;double atomN421[]={7.0,9.0,1.0};atomN=atomN421;
gd.input1(421,"C7H9N","2,4-dimethylpyridine",atomName,atomN);
gd.input2(107.156,0.0,431.6,647.0,0.0,0.0,0.0,0.0,2.3);
double aCPC421[]={0.0,0.0,0.0,0.0};aCPC=aCPC421;gd.input3(1,aCPC);
double aVPC421[]={10.2785,3991.27,-42.79,0.0};aVPC=aVPC421;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName422[]={"C","H","N"};atomName=atomName422;double atomN422[]={7.0,9.0,1.0};atomN=atomN422;
gd.input1(422,"C7H9N","2,5-dimethylpyridine",atomName,atomN);
gd.input2(107.156,0.0,430.2,644.2,0.0,0.0,0.0,0.0,2.2);
double aCPC422[]={0.0,0.0,0.0,0.0};aCPC=aCPC422;gd.input3(1,aCPC);
double aVPC422[]={9.6844,3545.14,-63.19,0.0};aVPC=aVPC422;gd.input4(3,aVPC);
gd.input5(66440.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName423[]={"C","H","N"};atomName=atomName423;double atomN423[]={7.0,9.0,1.0};atomN=atomN423;
gd.input1(423,"C7H9N","2,6-dimethylpyridine",atomName,atomN);
gd.input2(107.156,267.0,417.2,623.8,0.0,0.0,0.0,0.0,1.7);
double aCPC423[]={0.0,0.0,0.0,0.0};aCPC=aCPC423;gd.input3(1,aCPC);
double aVPC423[]={9.6286,3385.2,-65.19,0.0};aVPC=aVPC423;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName424[]={"C","H","N"};atomName=atomName424;double atomN424[]={7.0,9.0,1.0};atomN=atomN424;
gd.input1(424,"C7H9N","3,4-dimethylpyridine",atomName,atomN);
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gd.input2(107.156,0.0,452.3,683.8,0.0,0.0,0.0,0.0,1.9);
double aCPC424[]={0.0,0.0,0.0,0.0};aCPC=aCPC424;gd.input3(1,aCPC);
double aVPC424[]={10.3315,4237.04,-41.65,0.0};aVPC=aVPC424;gd.input4(3,aVPC);
gd.input5(70050.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName425[]={"C","H","N"};atomName=atomName425;double atomN425[]={7.0,9.0,1.0};atomN=atomN425;
gd.input1(425,"C7H9N","3,5-dimethylpyridine",atomName,atomN);
gd.input2(107.156,0.0,445.1,667.2,0.0,0.0,0.0,0.0,2.6);
double aCPC425[]={0.0,0.0,0.0,0.0};aCPC=aCPC425;gd.input3(1,aCPC);
double aVPC425[]={10.2648,4106.95,-44.45,0.0};aVPC=aVPC425;gd.input4(3,aVPC);
gd.input5(72810.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName426[]={"C","H","N"};atomName=atomName426;double atomN426[]={7.0,9.0,1.0};atomN=atomN426;
gd.input1(426,"C7H9N","p-toluidine",atomName,atomN);
gd.input2(107.156,316.9,473.7,667.0,23.8,0.0,0.0,0.443,1.6);
double aCPC426[]={0.0,0.0,0.0,0.0};aCPC=aCPC426;gd.input3(1,aCPC);
double aVPC426[]={10.0766,4041.04,-72.15,0.0};aVPC=aVPC426;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName427[]={"C","H","O"};atomName=atomName427;double atomN427[]={7.0,14.0,1.0};atomN=atomN427;
gd.input1(427,"C7H14O","methylamylketone",atomName,atomN);
gd.input2(114.188,0.0,424.2,611.5,34.4,0.0,0.0,0.483,0.0);
double aCPC427[]={0.0,0.0,0.0,0.0};aCPC=aCPC427;gd.input3(1,aCPC);
double aVPC427[]={0.0,0.0,0.0,0.0};aVPC=aVPC427;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName428[]={"C","H","O"};atomName=atomName428;double atomN428[]={7.0,14.0,2.0};atomN=atomN428;
gd.input1(428,"C7H14O2","isoamylacetate",atomName,atomN);
gd.input2(130.187,194.7,415.7,599.0,0.0,0.0,0.0,0.0,1.8);
double aCPC428[]={0.0,0.0,0.0,0.0};aCPC=aCPC428;gd.input3(1,aCPC);
double aVPC428[]={10.5011,3699.0,29.0,-57.54};aVPC=aVPC428;gd.input4(3,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName429[]={"C","H"};atomName=atomName429;double atomN429[]={7.0,16.0};atomN=atomN429;
gd.input1(429,"C7H16","2-methylhexane",atomName,atomN);
gd.input2(100.205,154.9,363.2,530.4,27.3,421.0,0.261,0.329,0.0);
double aCPC429[]={-39.39,0.8642,-6.289E-4,1.836E-7};aCPC=aCPC429;gd.input3(1,aCPC);
double aVPC429[]={-7.62477,1.47806,-3.53616,-2.70794};aVPC=aVPC429;gd.input4(1,aVPC);
gd.input5(195100.0,3220.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName430[]={"C","H","O"};atomName=atomName430;double atomN430[]={6.0,12.0,2.0};atomN=atomN430;
gd.input1(430,"C6H12O2A","n-amylformate",atomName,atomN);
gd.input2(116.16,199.7,403.6,576.0,34.6,1.0,0.0,0.538,0.0);
double aCPC430[]={0.0,0.0,0.0,0.0};aCPC=aCPC430;gd.input3(1,aCPC);
double aVPC430[]={0.0,0.0,0.0,0.0};aVPC=aVPC430;gd.input4(0,aVPC);
gd.input5(0.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName431[]={"C","H","N"};atomName=atomName431;double atomN431[]={5.0,11.0,1.0};atomN=atomN431;
gd.input1(431,"C5H11N","piperidine",atomName,atomN);
gd.input2(85.15,262.7,379.6,594.0,47.6,289.0,0.28,0.251,1.2);
double aCPC431[]={-53.07,0.6289,-3.358E-4,6.427E-8};aCPC=aCPC431;gd.input3(1,aCPC);
double aVPC431[]={-7.56707,2.15002,-3.8903,-3.70363};aVPC=aVPC431;gd.input4(1,aVPC);
gd.input5(-49030.0,0.0);
gi.addElement(gd);

gd=new Gas_Data();
String atomName432[]={"O","N","Ar","C"};atomName=atomName432;double atomN432[]={0.210792,0.784318,0.004691,0.000199};atomN=atomN432;
```

```
gd.input1(432,"O0.210792N0.784318Ar0.000199","air",atomName,atomN);
 //public void input2(double aMolWt,double aTfp,double aTb,double aTc,double aPc,double aVc,double aZc,double aOmega,double aDipm )
gd.input2(28.964196998240002,59.75,78.8,132.5303,37.86,74.9,0.2904118,0.033761,18546);
double aCPC432[]={-53.07,0.6289,-3.358E-4,6.427E-8};aCPC=aCPC432;gd.input3(1,aCPC);
double aVPC432[]={-7.56707,2.15002,-3.8903,-3.70363};aVPC=aVPC432;gd.input4(1,aVPC);
gd.input5(-2.19608,-2.15732);
double agair[][]={{25.723723715676222,19.99232995854758,0.28314685702856945,-32.123563652414404,81.609,320.0},
{28.464145354908172,-1.164021370197852,0.3544070926810084,7.221339061364784,320.0,560.0},
{21.5993133407992,15.96178021757258,3.702729423134984,-4.879905099986132,560.0,800.0},
{22.763154093261136,14.200122777831522,2.238217697646537,-4.138882058708922,800.0,1040.0},
{26.291542733030408,9.495754850645417,-3.6190562872951055,-2.3764205985187483,1040.0,1280.0},
{29.32668801072842,6.09562628686765,-10.676895214728951,-1.3096147306086523,1280.0,1520.0},
{35.756238622623776,0.5200939494405615,-36.26361030650734,0.05483269974851683,1520.0,1760.0},
{36.61845505106491,0.10389584492555426,-43.90420820516371,0.09261066332475583,1760.0,2000.0},
{36.722142723274146,0.1707474036168994,-47.29394876002523,0.05444575004512367,2000.0,2240.0},
{28.718713072181927,4.775628262021043,24.52714872698266,-0.6915132545822185,2240.0,2480.0},
{44.50889410501734,-3.747424006916667,-136.81017213224615,0.604367728762747,2480.0,2720.0},
{-4.47620387925482,19.670678053826023,499.76687671980466,-2.547160034230336,2720.0,3000.0},
{ 36.80001467  ,0.539029387  ,-68.51625884  ,-0.019466005  ,3000.0  ,3400.0},
{ 34.73738048  ,1.352059205  ,-28.97252153  ,-0.109752215  ,3400.0  ,3800.0},
{ 44.11953294  ,-1.935021718  ,-256.9434715  ,0.214865727  ,3800.0  ,4200.0},
{ 56.82352321  ,-5.691266046  ,-681.9669078  ,0.525617897  ,4200.0  ,4600.0},
{ 41.99997604  ,-1.194108295  ,-204.1940195  ,0.141815168  ,4600.0  ,5000.0}};
gd.inputCp(agair);
double avisiair[]={-6.817292346102759,
0.8830146457621001,
-0.0012026562883010277,
1.8188979789272164E-6,
-2.139383229883467E-9,
1.8402774246587077E-12,
-1.1171057320985713E-15,
4.622248887615039E-19,
-1.23508557862883E-22,
1.9160802839635E-26,
-1.3085837116957147E-30};
double akiair[]={-1.1953112202083283,
0.11696095661777868,
-1.1547782080793012E-4,
1.3578222517628758E-7,
-1.1382639273194056E-10,
6.297910653661441E-14,
-2.021143575127782E-17,
2.114010910016399E-21,
8.315126218826288E-25,
-3.1062549427817927E-28,
3.1655477973439176E-32};
gd.input_visc( avisiair);
gd.input_k(akiair);
double aVPC[]=new double[11];
aVPC[0] = 29260.646069271195;
aVPC[1] = -2259.8141617915153;
aVPC[2] = 69.5576674641975;
aVPC[3] = -1.0204131289345368;
aVPC[4] = 0.0053280120631002;
aVPC[5] = 3.941627291728819E-5;
aVPC[6] = -6.10051325610627E-7;
aVPC[7] = 7.069076830080271E-10;
aVPC[8] = 2.8442172696837997E-11;
aVPC[9] = -1.874464113039966E-13;
aVPC[10] = 3.754590185769442E-16;
gd.input4(4,aVPC);
gi.addElement(gd);

//Oxygen-Mono (O)-433
gd=new Gas_Data();
String atomName433[]={"O"};atomName=atomName433;double atomN433[]={1.0};atomN=atomN433;
gd.input1(433,"O","oxygenmono",atomName,atomN);
//public void input2(MolWt,Tfp,Tb,Tc,Pc,Vc,Zc,omega,Dipm )
gd.input2(15.9994,124.58,187.5,313.76,88.83,53.5,0.182217186,0.22170925788660753,0.0);
//double aCPC433[]={19.25,0.05213,1.197E-5,-1.132E-8};aCPC=aCPC433;gd.input3(1,aCPC);
//double aVPC433[]={-6.00435,1.1885,-0.83408,-1.22833};aVPC=aVPC433;gd.input4(1,aVPC);
```

```
gd.input5(249173.0,231736.0); //delHF DelGF at 298.15K
double agO[][]={{27.113243600372932,-28.002649515691253,-0.09763199549228598,36.63413358015812,100.0,300.0},
{21.954321565714615,-2.9537383224186757,0.5709587861955978,2.2050832095536284,300.0,500.0},
{20.95836117072303,-0.23453362832524766,0.9814929586424891,0.09333050928708024,500.0,900.0},
{20.797611811539575,-0.008921850739434314,1.2308276267522134,0.0030811156747886374,900.0,1300.0},
{20.72207688284937,0.04411550353434745,1.632316335158926,-0.007128650698173709,1300.0,1700.0},
{22.85064744314589,-1.5094521641350616,-10.268196308084946,0.3127140655713671,1700.0,2100.0},
{24.199601790028737,-2.138764357450759,-25.575848136906004,0.3851929597523652,2100.0,2500.0},
{18.94215056627358,0.6477561585201267,30.722520042181277,-0.032342228679118026,2500.0,2900.0},
{21.275851691551047,-0.49029887362566843,1.3617094640903697,0.12411382243821242,2900.0,3300.0},
{21.021999588677296,-0.32999984298165247,8.339973878366267E-6,0.0999999831574623,3300.0,3700.0},
{27.826648106741068,-2.5643153213152,-185.2204986088691,0.3056440006792665,3700.0,4100.0},
{20.460408778202847,0.019144718400194844,-10.125605301527218,0.05177794632131345,4100.0,4500.0},
{31.77417851718992,-3.021731585562175,-465.14052893212335,0.2797808693103802,4500.0,4900.0},
{35.59904595860383,-3.715667520848408,-721.4971365799445,0.306569087926232,4900.0,5300.0},
{-22.72757436084337,10.804326610354423,2077.6285006236844,-0.7113797097511636,5300.0,5700.0},
{-31.30889725585602,12.148089075699284,2851.5613870391776,-0.7563233625033865,5700.0,6000.0}};
gd.inputCp(agO);

//Hydroxyl (OH)-434
gd=new Gas_Data();
String atomName434[]={"O","H"};atomName=atomName434;double atomN434[]={1.0,1.0};atomN=atomN434;
gd.input1(434,"OH","hydroxyl",atomName,atomN);
gd.input2(17.0073,166.95,290.88,447.5,85.42,45.5,0.104458,0.514899394892434,0.0);
//double aCPC433[]={19.25,0.05213,1.197E-5,-1.132E-8};aCPC=aCPC433;gd.input3(1,aCPC);
//double aVPC433[]={-6.00435,1.1885,-0.83408,-1.22833};aVPC=aVPC433;gd.input4(1,aVPC);
gd.input5(38987.0,34277.0); //delHF DelGF at 298.15K
double agOH[][]={{33.95694253910982,-23.17067147184451,0.06651513030328551,32.19736029556229,100.0,300.0},
{30.26797507684289,-3.844682591159159,0.4542349940042376,3.974637244038461,300.0,500.0},
{29.666869071843415,-3.221817515547478,1.0662577314728687,4.1550929424472605,500.0,900.0},
{20.92399042646177,10.376016076190794,11.945671551519345,-1.818704479644749,900.0,1300.0},
{21.59661312395352,9.879567346282762,9.06993558361918,-1.7341406449072014,1300.0,1700.0},
{27.552294340699902,5.2129291686875385,-19.968814471085963,-0.7021947235099304,1700.0,2100.0},
{30.252900936275726,3.522952103545637,-40.20638255082803,-0.4057498869889187,2100.0,2500.0},
{34.77668883815137,1.15287119256328,-89.0425917810075,-0.05650815954518798,2500.0,2900.0},
{29.03214256239683,3.695301349300251,-1.3616180727233669,-0.37411412207628636,2900.0,3300.0},
{41.0594659718094,-1.2004824583551692,-217.34493432100413,0.1871391643482404,3300.0,3700.0},
{31.303833812181235,2.3435292625310518,3.423147316548569,-0.1758892283761697,3700.0,4100.0},
{42.2046536854478,-1.2346035656628123,-297.2856045251393,0.15477003531933783,4100.0,4500.0},
{33.72501630060919,1.244995372682238,-5.984246456552321E-4,-0.04999963074667549,4500.0,4900.0},
{34.23496160289019,1.014257425043152,10.034594087659672,-0.025891026321623253,4900.0,5300.0},
{56.519727633269845,-4.499476047474825,-1065.968991709066,0.3574713466427597,5300.0,5700.0},
{85.98004408022827,-10.976982664657463,-2851.284876988295,0.7562524353070696,5700.0,6000.0}};
gd.inputCp(agOH);
/*double avisOH[]={0.0,0.0,0.0};
double akiOH[]={0.0,0.0,0.0};
gd.input_visc( avisOH);
gd.input_k(akiOH);*/
gi.addElement(gd);

//Hydrogen-Mono (H)-435
gd=new Gas_Data();
String atomName435[]={"H"};atomName=atomName435;double atomN435[]={1.0};atomN=atomN435;
gd.input1(435,"H","hydrogenmono",atomName,atomN);
gd.input2(1.00794,14.0,20.3,33.0,12.9,64.3,0.303,-0.21932350231467115,0.0);
//double aCPC10[]={27.14,0.009274,-1.381E-5,7.645E-9};aCPC=aCPC10;gd.input3(1,aCPC);
//double aVPC10[]={-5.57929,2.60012,-0.85506,1.70503};aVPC=aVPC10;gd.input4(1,aVPC);
gd.input5(217999.0,203278.0);//delHF DelGF at 298.15K
double agH[][]={{20.78600000003579,-2.4703047048195125E-10,-1.556979010200628E-12,4.4655867513281294E-10,100.0,300.0},
{20.786,-0.0,0.0,-0.0,300.0,500.0},
{20.785999999435816,1.1125372558673235E-9,3.9877240953477097E-10,-6.024125844745859E-10,500.0,900.0},
{20.786000001781677,-2.190249897617117E-9,-3.3935454007877633E-9,7.501195476450939E-10,900.0,1300.0},
{20.78600004413201,-3.949789462541935E-8,-1.6075248951540484E-7,9.891993765242304E-9,1300.0,1700.0},
{20.786000080564456,-5.678907877278107E-8,-4.758770889432171E-7,1.1223022154358398E-8,1700.0,2100.0},
{20.786000379665534,-2.207725355326006E-7,-3.305429651753591E-6,3.602865736975677E-8,2100.0,2500.0},
{20.785999161529638,4.1504904268587394E-7,1.0091475740925011E-5,-5.769347852218818E-8,2500.0,2900.0},
{20.786001419835554,-6.11814904047925E-7,-2.2576564619932536E-5,7.405959991971421E-8,2900.0,3300.0},
{20.7860040700615,-1.552409242876826E-6,-8.26622760901873E-5,1.663802289959326E-7,3300.0,3700.0},
{20.785992204881286,2.6676408129711367E-6,1.9677338069154962E-4,-2.565668758827146E-7,3700.0,4100.0},
{20.786020751550463,-6.44004303776823E-6,-6.372356663386651E-4,5.617629655071869E-7,4100.0,4500.0},
{20.785972676762054,7.756464070379164E-6,0.0010030567097288013,-6.18963417488674E-7,4500.0,4900.0},
```

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{20.78600659097283,-1.7239775520501291E-6,-2.8506441108473854E-4,1.2677012953362603E-7,4900.0,5300.0},
{20.786,-0.0,0.0,-0.0,5300.0,5700.0},
{20.784701741479516,2.959728794547439E-4,0.07396829556225161,-1.8973543716107073E-5,5700.0,6000.0}};
gd.inputCp(agH);
//double avisiH2[]={2.20821838055369,0.506980026395776,-0.00138019011996754,3.33648388844839E-6,-4.91516640898999E-9,4.34474801305987E-
12,-2.25000324346063E-15,6.28027257836331E-19,-7.28348681229068E-23};
//double akiH2[]={-20.9811386435507,1.0769371545451,-0.00238706110811684,5.26186077214256E-6,-7.66004998358933E-9,6.96248035011081E-12,-
3.72842468870476E-15,1.0718592543995E-18,-1.27416628164376E-22};
//gd.input_visc( avisiH2);
//gd.input_k(akiH2);

gi.addElement(gd);


}
//Input of all gas data
public void gasnames()
{   gi=new Vector<Gas_Data>();
                String atomName[];
double atomN[];
data1();
data2();
data3();
String aName;
double aNN;
ierror=1;
Gas_Data gd=new Gas_Data();
int ngas=gi.capacity();
String names[]=new String[ngas];
String formulas[]=new String[ngas];
formulas=new String[ngas];
Enumeration<Gas_Data> n1=gi.elements();
int i=0;
while(n1.hasMoreElements())
{gd=n1.nextElement();names[i]=gd.aName;formulas[i]=gd.aFormula;i++;}
this.names=names;
this.formulas=formulas;
}

 public Gas_Data input(String gName)
{  gi=new Vector<Gas_Data>();
 String atomName[];
double atomN[];
data1();
data2();
data3();
int i;
String aName;
double aNN;
ierror=1;

Gas_Data gd=new Gas_Data();
Enumeration<Gas_Data> n1=gi.elements();
while(n1.hasMoreElements())
{gd=n1.nextElement();
  if (gd.aFormula.equals(gName)   ||  gd.aName.equals(gName) ) {ierror=0;break;}
}
return gd;
}
public double func(double a[],double x)
   {// this function calculates the value of
    // a polynomial
    int n=a.length;
    double ff;
    if(n!=0.0)
    { ff=a[n-1];
      for(int i=n-2;i>=0;i--)
      { ff=ff*x+a[i]; }
    }
    else
      ff=0;
```

```
    return ff;
    }
//viscosity low pressure polynomial curve fitting
public double viscosity_poly(double T)
{return func(xvis,T)*1e-7; }
//Thermal conductivity low pressure polynomial curve fitting
public double k_poly(double T)
{return func(xk,T)*1e-3; }
//viscosity low-high pressure Reichenberg method
 public double viscosity_Reichenberg(double T,double P)
 {//Pc in kPa T and Tc in degree Kelvin M molecular mass in kg/kmol
   //mu is dipole moment in deby
  double N0=6.02214076e26;// avagadro number    1/kmol
   double R=8314.46261815324; // Universal gas constant  J/(kmolK)
   double eps=0.01*Math.pow((R*Tc*N0*N0/(M*M*M*Pc*Pc*Pc*Pc)),(1.0/6.0));
   double Tr=T/Tc;
   double Pr=P/Pc;
   double mur=0.5246*mu*mu*Pc/(Tc*Tc);
   double FP0=0;
   if(mur<0.022 && mur>=0) FP0=1.0;
   else if(mur>=0.022 && mur<0.075) FP0=1.0+30.55*Math.pow((0.292-Zc),1.72);
   else FP0=1.0+30.55*Math.pow((0.292-Zc),1.72)*(0.96+0.1*(Tr-0.7));
   double FQ0=1.0;
   double Q=0;
   if(name.equals("H2"))
   {Q=0.76;FQ0=1.22*Math.pow(Q,0.15)*(1.0+0.00385*Math.pow(((Tr-12.0)*(Tr-12.0)),1.0/M)*(Tr-12.0)/Math.abs(Tr-12.0));}
   //else if (name.equals("he"))
   //{Q=1.38;FQ0=1.22*Math.pow(Q,0.15)*(1.0+0.00385*Math.pow(((Tr-12.0)*(Tr-12.0)),1.0/M)*(Tr-12.0)/Math.abs(Tr-12.0));}
   //else if(name.equals("d2"))
   //{Q=0.52;;FQ0=1.22*Math.pow(Q,0.15)*(1.0+0.00385*Math.pow(((Tr-12.0)*(Tr-12.0)),1.0/M)*(Tr-12.0)/Math.abs(Tr-12.0));}
   else
   {Q=0;FQ0=1.0;}
   double Z1=(0.807*Math.pow(Tr,0.618)-0.357*Math.exp(-0.449*Tr)+0.34*Math.exp(-4.058*Tr)+0.018)*FP0*FQ0;
   double eta0=Z1/eps;
   double Z2=Z1;
   double alpha=0;
   double beta=0;
   double a,b,c,d,e,f,a1,a2,b1,b2,c1,c2,d1,d2,f1,f2,gamma,delta,epsilon,xsi,Y;
   if(Tr<=1.0)
   {  alpha=3.262+14.98*Math.pow(Pr,5.508);
                 beta=1.390+5.746*Pr;
      Z2=0.6+0.76*Math.pow(Pr,alpha)+(6.99*Math.pow(Pr,beta)-0.6)*(1.0-Tr);
   }
   else if(Tr>=1  && Tr<40 &&  Pr>0  && Pr<=100.0)
   {a1=1.245e-3;a2=5.1726;gamma=-0.3286;
    b1=1.653;b2=1.2723;
    c1=0.4489;c2=3.0578;delta=-37.7332;
    d1=1.7368;d2=2.2310;epsilon=-7.6351;
    f1=0.9425;f2=-0.1853;xsi=0.4489;
    a=a1/Tr*Math.exp(a2*Math.pow(Tr,gamma));
    b=a*(b1*Tr-b2);
    c=c1/Tr*Math.exp(c2*Math.pow(Tr,delta));
    d=d1/Tr*Math.exp(d2*Math.pow(Tr,epsilon));
    e=1.3088;
    f=f1*Math.exp(f2*Math.pow(Tr,xsi));
    Z2=Z1*(1.0+a*Math.pow(Pr,e)/(b*Math.pow(Pr,f)+1.0/(1.0+c*Math.pow(Pr,d))));
   }
   Y=Z2/Z1;
   double FP=(1.0+(FP0-1.0)/(Y*Y*Y))/FP0;
   double lnY=Math.log(Y);
   double FQ=(1.0+(FQ0-1.0)*(1.0/Y-0.007*lnY*lnY*lnY*lnY))/FQ0;
   double eta=Z2*FP*FQ/eps;
   return eta;
 }
 //viscosity low pressure Lucas method
 public double viscosity_Lucas(double T)
 {//Enter Pc in kPa T and Tc in degree Kelvin M molecular mass in kg/kmol
   //mu is dipole moment in deby
  double N0=6.02214076e26;// avagadro number    1/kmol
   double R=8314.46261815324; // Universal gas constant  J/(kmolK)
   double eps=0.01*Math.pow((R*Tc*N0*N0/(M*M*M*Pc*Pc*Pc*Pc)),(1.0/6.0));
```

```
  double Tr=T/Tc;
  double mur=0.5246*mu*mu*Pc/(Tc*Tc);
  double FP=0;
  if(mur<0.022 && mur>=0) FP=1.0;
  else if(mur>=0.022 && mur<0.075) FP=1.0+30.55*Math.pow((0.292-Zc),1.72);
  else FP=1.0+30.55*Math.pow((0.292-Zc),1.72)*(0.96+0.1*(Tr-0.7));
  double eta=(0.807*Math.pow(Tr,0.618)-0.357*Math.exp(-0.449*Tr)+0.34*Math.exp(-4.058*Tr)+0.018)*FP/eps;
  return eta;
 }
//Viscosity low-high pressure Lucas method
 public double viscosity_Lucas(double T,double P)
{//P kPA  T degree K
double alpha1=1.9824e-3;
double alpha2=5.2683;
double a=-0.5767;
double beta1=1.6552;
double beta2=1.276;
double gamma1=0.1319;
double gamma2=3.7035;
double c=-79.8678;
double delta1=2.9496;
double delta2=2.919;
double d=-16.6169;
double Tr=T/Tc;
double Pr=P/Pc;
double A=alpha1/Tr*Math.exp(alpha2*Math.pow(Tr,a));
double B=A*(beta1*Tr-beta2);
double x1=Math.pow(Tr,c);
double x1a=1.0/Math.pow(Tr,Math.abs(c));
double x2=gamma2*x1;
double x3=Math.exp(x2);
double x4=gamma1/Tr;
double x5=x4*x3;
double C=gamma1/Tr*Math.exp(gamma2*Math.pow(Tr,c));
double D=delta1/Tr*Math.exp(delta2*Math.pow(Tr,d));
double vis0=0;
if(xvis.length==0)
{System.out.println("viscosity data is not available as polynomial curve fitting Lucas approach will be used");
 vis0=viscosity_Lucas(T);
}
 else
  vis0=viscosity_poly(T);
System.out.println("vis0="+vis0);
double mur=0.5246*mu*mu*Pc/Tc;
double Q=1.0-5.655*mur;
double ratio=1+Q*A*Math.pow(Pr,1.5)/(B*Pr+1.0/(1.0+C*Math.pow(Pr,D)));
double vis=vis0*ratio;
return vis;
}
//Thermal conductivity Methods
//Low pressure
//Method of Chung low pressure
 public double k_Chung(double T)
 {   double R=8.31446261815324; // Universal gas constant  J/(kmolK)
 double visc=viscosity_Lucas(T);
 double w=Omega;
 double Tr=T/Tc;
  double Cv;
  double Cp=Cp(T);
  if(mole) Cv=Cp(T)-R;
  else      Cv=Cp(T)*M-R;
  //kJ/(kmolK);
  double alpha=Cv/R-3.0/2.0;
  double beta=0.7862-0.7109*w+1.3168*w*w;
  double Z=2.0+10.5*Tr*Tr;
  double fi=1.0+alpha*((0.215+0.28288*alpha-1.061*beta+0.26665*Z)/(0.6366+beta*Z+1.061*alpha*beta));
  double k2=visc*Cv/(M*1.0e-3)*3.75*fi/(Cv/R);
  return k2;
 }
 //Method of Chung high pressure ro kmol/m^3
 public double k_Chung(double T,double ro)
```

```
 {   double R=8.31446261815324; // Universal gas constant  J/(kmolK)
 double v=1/ro;
 double visc=viscosity_Lucas(T);
 double Tr=T/Tc;
  double Cv;
  double Cp=Cp(T);
  if(mole) Cv=Cp(T)-R;
  else      Cv=Cp(T)*M-R;
  double Mp=M*1e-3;
  double y=Vc*1e-3/6.0/v;
  double G1=(1.0-0.5*y)/((1.0-y)*(1.0-y)*(1.0-y));
  double ai[]={2.4166,-5.0924e-1,6.6107,1.4543e1,7.9274e-1,-5.8634,9.1089e1};
  double bi[]={7.4824e-1,-1.5094,5.6207,-8.9139,8.2019e-1,1.2801e1,1.2811e2};
  double ci[]={-9.1858e-1,-4.9991e1,6.476e1,-5.6379,-6.9369e-1,9.5893,-5.4217e1};
  double di[]={1.2172e2,6.9983e1,2.7039e1,7.4344e1,6.3173,6.5529e1,5.2381e2};
 double B[]=new double[7];
 double mur=131.3*mu/Math.sqrt(Vc*Tc);
 for(int i=0;i<7;i++)
 {B[i]=ai[i]+bi[i]*w+ci[i]*mur*mur*mur*mur;}
  double G2=(B[0]/y*(1.0-Math.exp(-B[3]*y))+B[1]*G1*Math.exp(B[4]*y)+B[2]*G1)/(B[0]*B[3]+B[1]+B[2]);
  double q=3.586e-3*Math.sqrt(Tc/Mp)/Math.pow(Vc,(2.0/3.0));
   double alpha=Cv/R-3.0/2.0;
  double beta=0.7862-0.7109*w+1.3168*w*w;
  double Z=2.0+10.5*Tr*Tr;
  double fi=1.0+alpha*((0.215+0.28288*alpha-1.061*beta+0.26665*Z)/(0.6366+beta*Z+1.061*alpha*beta));
  double k2=31.2*visc*fi/Mp*(1.0/G2+B[5]*y)+q*B[6]*y*y*Math.sqrt(Tr)*G2;
  return k2;
 }
//Method of Ely and Hanley low pressure
 public double k_Ely(double T)
 {   double R=8.31446261815324; // Universal gas constant  J/(kmolK)
 double Mp=M*1e-3;
 double Tr=T/Tc;
  double Cv;
  Cv=Cp(T)-R;
  //kJ/(kmolK);
  double Tplus=0;
  if(Tr<=2) Tplus=Tr;
  else  Tplus=2;
  double teta=1.0+(w-0.011)*(0.56553-0.86276*Math.log(Tplus)-0.69852/Tplus);
  double fi=(1.0+(w-0.011)*(0.3856-1.1617*Math.log(Tplus)))*0.288/Zc;
  double f=Tc/190.4*teta;
  double h=Vc/99.2*fi;
  double T0=T/f;
  double eta0=0;
  double C[]={2.90774e6,-3.31287e6,1.6081e6,-4.3319e5,7.06248e4,-7.11662e3,4.32517e2,-1.44591e1,2.03712e-1};
  for(int n=1;n<=C.length;n++)
  {eta0+=C[n-1]*Math.pow(T0,(n-4.0)/3.0);}
  eta0*=1.0e-7;
  double k0=1944.0*eta0;
  double H=Math.sqrt(16.04e-3/Mp)*Math.sqrt(f)/Math.pow(h,(2.0/3.0));
  double kstar=k0*H;
  double etastar=eta0*H*Mp/16.04e-3;
  double k=kstar+etastar/Mp*1.32*(Cv-3.0*R/2.0);
  return k;
 }
//Method of Ely and Hanley high pressure
 public double k_Ely(double T,double ro)
 {   double R=8.31446261815324; // Universal gas constant  J/(kmolK)
 double Mp=M*1e-3;
 double Tr=T/Tc;
  double Cv;
  double v=1.0/ro;
  double vr=v/(Vc*1e-3);
  Cv=Cp(T)-R;
  //kJ/(kmolK);
  double Tplus=0;
  if(Tr<=2) Tplus=Tr;
  else  Tplus=2;
  double vplus=0;
  if(vr>0.5 && vr<2) vplus=vr;
```

```
  else if(vr<=0.5) vplus=0.5;
  else vplus=2;
  double teta=1.0+(w-0.011)*(0.09057-0.86276*Math.log(Tplus)+(0.31664-0.46568/Tplus)*(vplus-0.5));
  double fi=(1.0+(w-0.011)*(0.3949*(vplus-1.02355)-0.93281*(vplus-0.75464)*Math.log(Tplus)))*0.288/Zc;
  double f=Tc/190.4*teta;
  double h=Vc/99.2*fi;
  double T0=T/f;
  double ro0=16.04*1e-3/v*h;
  double eta0=0;
  double C[]={2.90774e6,-3.31287e6,1.6081e6,-4.3319e5,7.06248e4,-7.11662e3,4.32517e2,-1.44591e1,2.03712e-1};
  for(int n=1;n<=C.length;n++)
  {eta0+=C[n-1]*Math.pow(T0,(n-4.0)/3.0);}
  eta0*=1.0e-7;
  double k1=1944.0*eta0;
  double b[]={2.5276e-4,3.3433e-4,1.12,1.68e2};
  double a[]={-7.19771,85.67882,12.47183,-984.6252,0.3594685,69.79841,-872.8833};
  double x1=b[2]-Math.log(T0/b[3]);
  double k2=(b[0]+b[1]*x1*x1)*ro0;
  double k3=Math.exp(a[0]+a[1]/T0)*
  (Math.exp((a[2]+a[3]/Math.pow(T0,(3.0/4.0)))*Math.pow(ro0,0.1)+(ro0/0.1617-1)*Math.sqrt(ro0)*(a[4]+a[5]/T0+a[6]/(T0*T0)))-1.0)-1.0e-3;
  double H=Math.sqrt(16.04e-3/Mp)*Math.sqrt(f)/Math.pow(h,(2.0/3.0));
  double kstar=(k1+k2+k3)*H;
  double etastar=eta0*H*Mp/16.04e-3;
  double k=kstar+etastar/Mp*1.32*(Cv-3.0*R/2.0);
  return k;
 }
 public double Cp(double T)
 { double Cp=0;
 if( aCpEq==1)
   {Cp=func(aCPC,T);}
  else if( aCpEq==2)
   {
      for (int i=0;i<n_equation;i++)
        {  if((T <= th[i]) && (T >= tl[i]) )
                        Cp=xa[i]+xb[i]*1.0e-3*T+xc[i]*1.0e5/T/T+xd[i]*1.0e-6*T*T;
                    }
   }
    if(!mole) Cp/=M;
 return Cp;
 }
   public double h1(double T)
   {    double hh =0;
                if( aCpEq==1)
   { hh=aCPC[0]*T+aCPC[1]*T*T/2.0+aCPC[2]*T*T*T/3.0+aCPC[3]*T*T*T*T/4.0;}
    else if( aCpEq==2)
   {
   //  enthalpy KJ/kmol
   //integration of function dh=Cp(T)*dT

     for(int i=0;i<n_equation;i++)
     {
                    if(((T>th[i]) && (i== (n_equation-1) ) )
                                || ((T<tl[i]) && (i== 0 ) ) )
            {
                    hh+=   xa[i]*(T- tl[i])
                        + xb[i]*1.0e-3/2.0*(T*T-tl[i]*tl[i])
                                - xc[i]*1e5*(1/T-1/tl[i])
                                + xd[i]*1e-6*(T*T*T-tl[i]*tl[i]*tl[i])/3.0;
      }
            else if((T<= th[i]) && (T> tl[i]))
                                                        {
                    hh+=   xa[i]*(T- tl[i])
                        + xb[i]*1.0e-3/2.0*(T*T-tl[i]*tl[i])
                                - xc[i]*1e5*(1/T-1/tl[i])
                                + xd[i]*1e-6*(T*T*T-tl[i]*tl[i]*tl[i])/3.0;
            }
            else if(T>th[i])
                                                        {
                    hh+=   xa[i]*(th[i]- tl[i])
                        + xb[i]*1.0e-3/2.0*(th[i]*th[i] - tl[i]*tl[i])
                                - xc[i]*1e5*(1/th[i]-1/tl[i])
```

```
                                + xd[i]*1e-6*(th[i]*th[i]*th[i]-tl[i]*tl[i]*tl[i])/3.0;
          }
                }
  }
   if(!mole) hh/=M;
   return hh;
   }

   public double h(double T)
   {return h1(T)-h1(273.15);}

    public double u1(double T)
   {    double uu=h1(T)-R*1e-3*T;
        return uu;
   }

     public double u(double T)
   {return u1(T)-u1(273.15);}

    // integral Cv/T
    public double s2(double T)
    {double ss=s1(T)-R*1e-3*Math.log(T); return ss;}
    // integral Cp/T
   public double s1(double T)
   { double ss =0;
                if( aCpEq==1)
   { ss=aCPC[0]*Math.log(T)+aCPC[1]*T+aCPC[2]*T*T/2.0+aCPC[3]*T*T*T/3.0;}
    else if( aCpEq==2)
   {
   //entropy KJ/kmol K
   //integration of function
   // ds = Cp(T) * dt/T - R dP/P
   // 0 point at 0 K (so is added up at 298 K)
   for(int i=0;i<n_equation;i++)
                                {
         if( ( T > th[i]  && i==n_equation - 1 )
                    | | ( T < tl[i]  && i==0            ))
                                    {
                      ss+=xa[i]*Math.log(T/tl[i])
                      + xb[i]*1.0E-3*(T-tl[i])
                      - xc[i]*1e5/2.0*(1.0/(T*T) - 1.0/(tl[i]*tl[i]))
                      + xd[i]*1e-6/2.0*(T*T-tl[i]*tl[i]);
            }
                   else if((T <= th[i]) && (T > tl[i]))
                      {
                      ss+=xa[i]*Math.log(T/tl[i])
                      + xb[i]*1.0E-3*(T-tl[i])
                      - xc[i]*1e5/2.0*(1.0/(T*T) - 1.0/(tl[i]*tl[i]))
            + xd[i]*1e-6/2.0*(T*T-tl[i]*tl[i]);
                                                                    }
                   else if( T > th[i] )
                      {
                      ss+=xa[i]*Math.log(th[i]/tl[i])
                      + xb[i]*1.0E-3*(th[i]-tl[i])
                      - xc[i]*1e5/2.0*(1.0/(th[i]*th[i]) - 1.0/(tl[i]*tl[i]))
                      + xd[i]*1e-6/2.0*(th[i]*th[i] - tl[i]*tl[i]);
                                                                    }
                   }
   }
   if(!mole) ss/=M;
   return ss;
   }

    public double s(double T)
   {return s1(T)-s1(T0);}

//vapor pressure kPa;
public double Ps(double T)
{  double Ps=0;
double y=0;
                if(aVPEq==1)
```

```
    {double x=1.0-T/Tc;
    double x3=x*x*x;
     y=1.0/(1.0-x)*(aVPC[0]*x+aVPC[1]*Math.pow(x,1.5)+aVPC[2]*x3+aVPC[3]*x3*x3);
     Ps=Pc*Math.exp(y)*100.0;
    }
    else if(aVPEq==2)
    {y=aVPC[0]-aVPC[1]/T+aVPC[2]*Math.log(T)+aVPC[3]/(T*T);
     Ps=Math.exp(y)*100.0;
    }
    else if(aVPEq==3)
    {y=aVPC[0]-aVPC[1]/(T+aVPC[2]);
     Ps=Math.exp(y)*100.0;
    }
    else if(aVPEq==4)
    {Ps=func(aVPC,T);}
      return Ps;
}
public double viscosity(double T)
{  double vis0=0;
                if(xvis.length==0)  { vis0=viscosity_Lucas(T);}
 else {vis0=viscosity_poly(T);}
 return vis0;
}
public double k(double T)
{double k0=0;
  if(xk.length==0)  { k0=k_Chung(T);}
 else {k0=k_Ely(T);}
 return k0;
}
/*
//Method of Pitzer, acentric factor estimation
 public double w_pitzer(double Tb,double Tc, double Pc)
 {   //P bar  T degree K
                double w_pitzer=0;
                double Tbr=Tb/Tc; double Tr=Tbr;
                double to=(1-Tr);
                double f0=(-5.97616*to + 1.29874*Math.pow(to,1.5) - 0.60394*Math.pow(to,2.5) - 1.06841*Math.pow(to,5)) / Tr;
                double f1=(-5.03365*to + 1.11505*Math.pow(to,1.5) - 5.41217*Math.pow(to,2.5) - 7.46628*Math.pow(to,5)) / Tr;

                w_pitzer= -( Math.log(Pc/1.01325) + f0 ) /f1;

  return w_pitzer;
 }
*/
public static void main(String arg[])
{Gas_Data gd=new Gas_Data();
   gd.gasnames();
    String c[][]={gd.names,gd.formulas};
    String s[]={"Names","Formulas"};
    //Text.printT(c,s,"Gas List");
  gd=gd.input("air");
    double T=298.15;
  double P=100; //kpa
  System.out.println(gd.aFormula+"
M="+gd.aMolWt+"Tc="+gd.Tc+"Pc="+gd.Pc+"Vc="+gd.Vc+"Zc="+gd.Zc+"w="+gd.w+"Cp="+gd.Cp(T)+"h="+gd.h(298.15)+"s="+gd.s(298.15));

  Gas_PR1 pr=new Gas_PR1("air");
  double v=pr.v(T,P);
  double ro=1.0/v;
  System.out.println("ro="+ro);
  System.out.println("v="+v);
 // System.out.println("vis1="+gd.viscosity_poly(T)+"vis1="+gd.viscosity_Lucas(T,P)+"vis2="+gd.viscosity_Reichenberg(T,P));
  System.out.println("k1="+gd.k_poly(T)+"k2="+gd.k_Chung(T)+"k3="+gd.k_Ely(T));
  //System.out.println("Pc="+gd.Pc+"Ps(100)="+gd.Ps(100.0));
  double k2=gd.k_Chung(T,1.0/v);
   double k3= gd.k_Ely(T,1.0/v);
      System.out.println("k2="+k2+"k3="+k3);
}
}
```

Gas_PG

```
import java.io.*;
import javax.swing.*;
public class Gas_PG
{public Gas_Data gd;
 boolean mole=true;
 public double M;
 public double R; // Universal gas constant  J/(kmolK)
 Atom atomList[];
 int natom;
 String Formula;
 String Name;
 double mu0=0;
 double P0=101.325; //kP
 double T0=273.15;
   double v0,ro0,v0M;
  public double Tfp,Tb,Tc,Pc,Vc,roc,Zc,Omega,mu;
 public Gas_PG(String gas_name)
 {  gas_name=gas_name.toUpperCase();
                gd=new Gas_Data();
  gd=gd.input(gas_name);
  M=gd.M;
  R=8314.46261815324;
  natom=gd.atomName.length;
  atomList=new Atom[natom];
  Formula=gd.aFormula;
  Name=gd.aName;
   M=gd.M;
  Tfp=gd.Tfp;
  Tb=gd.Tb;
  Tc=gd.Tc;
  Vc=gd.aVc;
  roc=1.0/Vc;
  Pc=gd.Pc;
  Zc=gd.aZc;
  for(int i=0;i<natom;i++)
 {atomList[i]=new Atom(gd.atomName[i],gd.atomN[i]);
  //System.out.println(gd.name+" "+gd.atomName[i]+" "+gd.atomN[i]);
 }
  }

  public double Cp(double T)
  {double Cp=gd.Cp(T);
   if(!mole) Cp/=M;
   return Cp;
  }

  public double Cv(double T)
  {double Cp=gd.Cp(T);
   double Cv=Cp-R*1e-3;
   if(!mole) Cv/=M;
   return Cv;
  }
   public double integCv(double T)
{ double iCv=gd.u1(T);
   if(!mole)  iCv/=M;
  return iCv;
}
public double integCp_T(double T)
{  double iCp=gd.s1(T);
    if(!mole)  iCp/=M;
    return iCp;
}
 public double integCp(double T)
{ double iCp=gd.h1(T);
   if(!mole)  iCp/=M;
  return iCp;
}
public double integCv_T(double T)
{  double iCv=gd.s2(T);
```

```
    if(!mole)  iCv/=M;
    return iCv;
}
  public double h(double T)
  { double h=gd.h(T);
    if(!mole) h/=M;
    return h;
  }

  public double ht(double T)
  {double h=gd.h(T)-gd.h(298.15)+gd.aDELHF;
    if(!mole) h/=M;
    return h;
  }

  public double u(double T)
  {double h=gd.h(T);
  double T0=273.15;
    double u=h-R*1.0e-3*(T-T0);
    if(!mole) u/=M;
    return u;
  }
   public double st(double T,double P)
  {  double dS=gd.aDELSF;
      if(!mole) dS/=M;
                double s0t=s(T,P)-s(298.15,P)+dS;
    return s0t;
  }
   public double s0t(double T)
  { return st(T,P0);}

   public double s(double T,double P)
  { double s=gd.s(T)-gd.s(T0)-R*1e-3*Math.log(P/P0);
    if(!mole) s/=M;
    return s;
  }
public double s(double T)
{return s(T,P0)-s(T0,P0);}

public double s0(double T)
{return s(T);}

  public double P_Tv(double T,double v)
  {double P=R*T/v;
    if(!mole) P/=M;
    return P*1e-3;  //kPa
  }

  public double P_Tro(double T,double ro)
  {double P=R*T*ro;
    if(!mole) P/=M;
    return P*1e-3; //kPa
  }

  public double T_Pro(double P,double ro)
 {double T=P*1e3/(R*ro); //case of ideal gas
   if(!mole)  T/=M;
   return T;
  }
 public double T_h(double h)
{if_x f1=x->h(x)-h;
 double T=secant(f1,T0);
 return T;
}

public double T_sP(double s,double P)
{if_x f1=x->s(x,P)-s;
 double T=secant(f1,T0);
 return T;
}
```

```
public double P_Ts(double T,double s)
{if_x f1=x->s(T,x)-s;
 double P=secant(f1,P0);
 return P;
}

    public double T_Pv(double P,double v)
 {double T=P*1e3*v/R; //case of ideal gas
   if(!mole)  T/=M;
   return T;
  }
  public double v(double T,double P)
  {double v=R*T/(P*1.0e3);
      if(!mole) v/=M;
      return v;
  }

   public double ro(double T,double P)
  {double v=R*T/(P*1.0e3);
     if(!mole) v/=M;
    double ro=1.0/v;
      return ro;
  }


  //Gibbs free energy
  public double g(double T,double P)
{ return h(T)-T*s(T,P);
}

public double gt(double T,double P)
{ return ht(T)-T*st(T,P);}

public double gt0(double T)
{ return ht(T)-T*s0(T);}


  public double viscosity(double T)
  {return gd.viscosity(T);}

   public double k(double T)
  {return gd.k(T);}

public double Prandtl(double T)
{
// Prandtl number
double Cp=0;
if(mole) {Cp=Cp(T)/M;}
else {Cp=Cp(T);}
double Pr=0;
Pr=Cp*1.0e3*viscosity(T)/k(T);
return Pr;
}
double beta(double T,double ro)
{return 1.0/T;}

//Isothermal compresibility
public double dP_dv_Tro(double T,double ro)
{double v=1.0/ro;
 double v1=0;
 if(!mole) v1=v*M;
 else v1=v;
 double y=-R*T/(v1*v1);
 return y;
}
public double kappaS_Tro(double T,double ro)
{  double y1=dP_dv_Tro(T,ro);
   double v=1.0/ro;
    double v1=0;
    if(!mole) v1=v*M;
    else v1=v;
```

```
   double y=-1.0/y1/v1;
  return y;
}
//Isothermal compresibility
public double kappaS_TP(double T,double P)
{  double v=v(T,P);
   double ro=1.0/v;
   double y1=dP_dv_Tro(T,ro);
    double v1=0;
    if(!mole) v1=v*M;
    else v1=v;
   double y=-1.0/y1/v1;
  return y;
}
//speed of sound
public double a_T(double T)
{  double gamma=Cp(T)/Cv(T);
   double x=gamma*R/M*T;
   double a=Math.sqrt(x);
   return a;
}
public double w_T(double T)
{  double gamma=Cp(T)/Cv(T);
   double x=gamma*R/M*T;
   double a=Math.sqrt(x);
   return a;
}
public static double[] secant2(ifi_xj f,double x[])
{
// Roots of nonlinear system of equations secant method
//ti : weight function
//x vector of independent variables
//y vector of dependent variables
//dy derivative vector of dependent variables
double ti=1.0;
int i;
int nmax=20;
double tolerance=1.0e-4;
int n=x.length;
double b[];
b=new double[n];
for(i=0;i<n;i++)
{
b[i]=1.0;
}
i=0;
while( i++ < nmax && Matrix.abs(b) > tolerance )
{ b=Matrix.multiply(Matrix.divide(f.func(x),f.dfunc(x)),-ti);
  x=Matrix.add(x,b);
}
if(i >= nmax) System.out.println("Warning : Maximum number of iterations are exceeded \nResults may not be valid");
return x;
}
 public static double secant(if_x f,double x)
{ double eps=1.0e-6;
  double y=f.func(x);
  double dy=f.dfunc(x);
  int miter=100;
  int i=0;
  while(Math.abs(y)>eps && i<miter)
  {x=x-y/dy;
   y=f.func(x);
   dy=f.dfunc(x);
   i++;
  }
  if(i>=miter)
    System.out.println("i="+i+"result may not be correct");
  return x;
}
public double[] property_TP(double T,double P)
{double a[]=new double[17];
```

```
 double ro=ro(T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Pro(double P,double ro)
{double a[]=new double[17];
 double T=T_Pro(P,ro);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Tro(double T,double ro)
{double a[]=new double[17];
 double P=P_Tro(T,ro);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Ph(double P,double h)
{double a[]=new double[17];
 double T=T_h(h);
 double ro=ro( T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
```

```
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Ps(double P,double s)
{double a[]=new double[17];
 double T=T_sP(s,P);
 double ro=ro( T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
public double[] property_Ts(double T,double s)
{double a[]=new double[17];
 double P=P_Ts(T,s);
 double ro=ro( T,P);
 a[1]=T;
 a[2]=1.0/ro;
 a[0]=P;
 a[3]=h(T);
 a[4]=u(T);
 a[5]=s(T,P);
 a[6]=2.0;
 a[7]=Cp(T);
 a[8]=Cv(T);
 a[9]=beta(T,ro);
 a[10]=kappaS_Tro(T,ro);
 a[11]=viscosity(T);
 a[12]=k(T);
 a[13]=0.0;
 a[14]=Prandtl(T);
 a[15]=ro;
 a[16]=w_T(T);
 return a;
}
        public double mu(double iT,double iP,double n,double nt){
                double mu=0;
                        double value=0;
                        double lnP=Math.log(iP/P0);
                        value=Math.abs(n)<1e-20? 0 :Math.log(n/nt);
                        mu=(gt(iT,P0)+8.3145*iT*value+8.3145*iT*lnP);
                return mu;
        }
        public void getmu0(double iT,double iP){
```

```
                    mu0=gt0(iT);
            }
  public double[] property(String s,double v1,double v2)
{ if(s.equals("pt")) return property_TP(v2,v1);
  else if(s.equals("tp"))  {return property_TP(v1,v2);}
  else if(s.equals("vt"))  {double ro=1.0/v1;return property_Tro(v2,ro);}
  else if(s.equals("tv"))  {double ro=1.0/v2;return property_Tro(v1,ro);}
  else if(s.equals("rot")) {return property_Tro(v2,v1);}
  else if(s.equals("tro")) {return property_Tro(v1,v2);}
  else if(s.equals("pv"))  return property_Pro(v1,1.0/v2);
  else if(s.equals("pro")) return property_Pro(v1,v2);
  else if(s.equals("vp"))  return property_Pro(v2,1.0/v1);
  else if(s.equals("rop")) return property_Pro(v2,v1);
  else if(s.equals("ph"))  return property_Ph(v1,v2);
  else if(s.equals("hp"))  return property_Ph(v2,v1);
  else if(s.equals("ps"))  return property_Ps(v1,v2);
  else if(s.equals("sp"))  return property_Ps(v2,v1);
  //else if(s.equals("ts"))  return property_Ts(v1,v2);
  //else if(s.equals("st"))  return property_Ts(v2,v1);
  else return property_TP(v1,v2);
}
public double[] propertyC(String s,double v1,double v2)
{ double t=273.15;
  if(s.equals("pt")) return property_TP(v2,(v1+t));
  else if(s.equals("tp"))  {return property_TP((v1+t),v2);}
  else if(s.equals("vt"))  {double ro=1.0/v1;return property_Tro((v2+t),ro);}
  else if(s.equals("tv"))  {double ro=1.0/v2;return property_Tro((v1+t),ro);}
  else if(s.equals("rot")) {return property_Tro((v2+t),v1);}
  else if(s.equals("tro")) {return property_Tro((v1+t),v2);}
  else if(s.equals("pv"))  return property_Pro(v1,1.0/v2);
  else if(s.equals("pro")) return property_Pro(v1,v2);
  else if(s.equals("vp"))  return property_Pro(v2,1.0/v1);
  else if(s.equals("rop")) return property_Pro(v2,v1);
  else if(s.equals("ph"))  return property_Ph(v1,v2);
  else if(s.equals("hp"))  return property_Ph(v2,v1);
  else if(s.equals("ps"))  return property_Ps(v1,v2);
  else if(s.equals("sp"))  return property_Ps(v2,v1);
  else return property_TP((v1+t),v2);
}
public boolean input1()
{   Object[] o=new Object[]{"tp","vt","tv","rot","tro","pv","pro","vp","rop","ph","hp","ps","sp","quit"};
    String oname[]=new String[2];
    double v[]=new double[3];
    boolean b=true;
    ImageIcon picture=null;//new ImageIcon("fall.jpg");
    String option=(String)JOptionPane.showInputDialog(null,"Please select a known pair : ",
    "Input parameters of dry air ideal gas EOS",JOptionPane.QUESTION_MESSAGE,picture,o,"ATP");
     if(option.equals("tp")) {oname[0]="Temperature degree C";oname[1]="Pressure kPa";}
     else if(option.equals("vt")) {oname[1]="Temperature degree C";oname[0]="specific volume m^3/kg";}
     else if(option.equals("tv")) {oname[1]="Temperature degree C";oname[0]="specific volume m^3/kg";}
     else if(option.equals("rot")) {oname[1]="Temperature degree C";oname[0]="density kg/m^3";}
     else if(option.equals("tro")) {oname[0]="Temperature degree C";oname[1]="density kg/m^3";}
     else if(option.equals("pv")) {oname[0]="Pressure kPa";oname[1]="specific volume m^3/kg";}
     else if(option.equals("pro")) {oname[0]="Pressure kPa";oname[1]="density kg/m^3";}
     else if(option.equals("vp")) {oname[1]="Pressure kPa";oname[0]="specific volume m^3/kg";}
     else if(option.equals("rop")) {oname[1]="Pressure kPa";oname[0]="density kg/m^3";}
     else if(option.equals("ph")) {oname[0]="Pressure kPa";oname[1]="h enthalpy kJ/kg";}
     else if(option.equals("hp")) {oname[1]="Pressure kPa";oname[0]="h enthalpy kJ/kg";}
     else if(option.equals("ps")) {oname[0]="Pressure kPa";oname[1]="s entropy kJ/kgK";}
     else if(option.equals("sp")) {oname[1]="Pressure kPa";oname[0]="s entropy kJ/kgK";}
     else b=false;
    if(b)
    {
    for(int i=0;i<2;i++)
            {v[i] =Double.parseDouble(JOptionPane.showInputDialog(oname[i]));}
    print(option,v[0],v[1]);
    }
   return b;
}
public String toString()
{
```

```
//return the chemical symbol of the gas
String s="";
for(int i=0;i<natom;i++)
  s=s+atomList[i].toString();
return s;
}
public void printC(String s,double v1,double v2)
{String s1[][]=toStringC(s,v1,v2);
 String s3="Properties of dry air ideal gas EOS ";
 String s2[]={"array no","property name","dry air property","unit"};
 Text.print(s1,s2,s3);
}
public void print(String s,double v1,double v2)
{String s1[][]=toString(s,v1,v2);
 String s3="Properties of dry air ideal gas EOS ";
 String s2[]={"array no","property name","dry air property","unit"};
 Text.print(s1,s2,s3);
}
public String[][] toString(String s, double v1, double v2)
{  String s1[][]=new String[17][4];
   s1[0][1]="P, pressure       ";
   s1[1][1]="T, temperature     ";
   s1[2][1]="v, specific volume ";
   s1[3][1]="h, enthalpy       ";
   s1[4][1]="u, internal energy ";
   s1[5][1]="s, entropy        ";
   s1[6][1]="x, quality        ";
   s1[7][1]="Cp, specific heat at constant pressure ";
   s1[8][1]="Cv, specific heat at constant volume ";
   s1[9][1]=""+'\u03B1'+" isobaric thermal expansion coefficient ";
   s1[10][1]=""+'\u03BA'+" isothermal compressibility" ;
   s1[11][1]=""+'\u03B7'+" Dynamic viscosity" ;
   s1[12][1]="k Thermal conductivity" ;
   s1[13][1]=""+'\u03C3'+" Surface tension" ;
   s1[14][1]="Prandtl number" ;
   s1[15][1]=""+'\u03C1'+" density" ;
   s1[16][1]=" speed of sound" ;
   if(!mole)
   {
   s1[0][3]=" kPA         ";
   s1[1][3]=" deg K        ";
   s1[2][3]=" m"+'\u00B3'+"/kg       ";
   s1[3][3]=" KJ/kg        ";
   s1[4][3]=" KJ/kg        ";
   s1[5][3]=" KJ/kgK        ";
   s1[6][3]=" kg vap/kg mix ";
   s1[7][3]=" KJ/kgK";
   s1[8][3]=" KJ/kgK";
   s1[9][3]=" 1/K";
   s1[10][3]=" 1/Pa";
   s1[11][3]=" Pa.s";
   s1[12][3]=" W/mK";
   s1[13][3]=" N/m";
   s1[14][3]=" ";
   s1[15][3]=" kg/m"+'\u00B3';
   s1[16][3]=" m/s";
   }
   else{
   s1[0][3]=" kPA         ";
   s1[1][3]=" deg K        ";
   s1[2][3]=" m"+'\u00B3'+"/kmol       ";
   s1[3][3]=" KJ/kmol        ";
   s1[4][3]=" KJ/kmol        ";
   s1[5][3]=" KJ/kmolK        ";
   s1[6][3]=" kg vap/kg mix ";
   s1[7][3]=" KJ/kmolK";
   s1[8][3]=" KJkmolK";
   s1[9][3]=" 1/K";
   s1[10][3]=" 1/Pa";
   s1[11][3]=" Pa.s";
   s1[12][3]=" W/mK";
```

```
  s1[13][3]=" N/m";
  s1[14][3]=" ";
  s1[15][3]=" kmol/m"+'\u00B3';
  s1[16][3]=" m/s";
  }
 double pp[]=property(s,v1,v2);
for(int i=0;i<17;i++)
  {s1[i][2]=""+pp[i];}
   //s1[6][2]=phase(pp[6]);
for(int i=0;i<17;i++)
{s1[i][0]=""+i;}
return s1;
}
public String[][] toStringC(String s, double v1, double v2)
{  String s1[][]=new String[17][4];
  s1[0][1]="P, pressure       ";
  s1[1][1]="T, temperature     ";
  s1[2][1]="v, specific volume ";
  s1[3][1]="h, enthalpy       ";
  s1[4][1]="u, internal energy ";
  s1[5][1]="s, entropy        ";
  s1[6][1]="x, quality        ";
  s1[7][1]="Cp, specific heat at constant pressure ";
  s1[8][1]="Cv, specific heat at constant volume ";
  s1[9][1]=""+'\u03B1'+" isobaric thermal expansion coefficient ";
  s1[10][1]=""+'\u03BA'+" isothermal compressibility" ;
  s1[11][1]=""+'\u03B7'+" Dynamic viscosity" ;
  s1[12][1]="k Thermal conductivity" ;
  s1[13][1]=""+'\u03C3'+" Surface tension" ;
  s1[14][1]="Prandtl number" ;
  s1[15][1]=""+'\u03C1'+" density" ;
  s1[16][1]=" speed of sound" ;
  if(!mole)
  {
  s1[0][3]=" kPA         ";
  s1[1][3]=" deg K        ";
  s1[2][3]=" m"+'\u00B3'+"/kg       ";
  s1[3][3]=" KJ/kg        ";
  s1[4][3]=" KJ/kg        ";
  s1[5][3]=" KJ/kgK        ";
  s1[6][3]=" kg vap/kg mix ";
  s1[7][3]=" KJ/kgK";
  s1[8][3]=" KJ/kgK";
  s1[9][3]=" 1/K";
  s1[10][3]=" 1/Pa";
  s1[11][3]=" Pa.s";
  s1[12][3]=" W/mK";
  s1[13][3]=" N/m";
  s1[14][3]=" ";
  s1[15][3]=" kg/m"+'\u00B3';
  s1[16][3]=" m/s";
  }
  else{
  s1[0][3]=" kPA         ";
  s1[1][3]=" deg K        ";
  s1[2][3]=" m"+'\u00B3'+"/kmol       ";
  s1[3][3]=" KJ/kmol        ";
  s1[4][3]=" KJ/kmol        ";
  s1[5][3]=" KJ/kmolK        ";
  s1[6][3]=" kg vap/kg mix ";
  s1[7][3]=" KJ/kmolK";
  s1[8][3]=" KJkmolK";
  s1[9][3]=" 1/K";
  s1[10][3]=" 1/Pa";
  s1[11][3]=" Pa.s";
  s1[12][3]=" W/mK";
  s1[13][3]=" N/m";
  s1[14][3]=" ";
  s1[15][3]=" kmol/m"+'\u00B3';
  s1[16][3]=" m/s";
  }
```

```
  double pp[]=propertyC(s,v1,v2);
for(int i=0;i<17;i++)
   {s1[i][2]=""+pp[i];}
    //s1[6][2]=phase(pp[6]);
for(int i=0;i<17;i++)
{s1[i][0]=""+i;}
return s1;
}

public static void main(String arg[])
{Gas_PG pr=new Gas_PG("N2");
  double T=1000; //degree K
  double P=100.0; //kPa
  pr.print("tp",T,P);
  double a[]=pr.property("tp",T,P);
  for( double x :a) System.out.println(x);
}
}
```

Atom.java

```
//=====================================================
// Thermodynamic Package in java
// Class Atom
// Properties of single atom
// ---------------------------------------------------
// Dr. M. Turhan Coban
// Ege University, school of Engineering, Department of Mechanical Engineering
// email : turhan_coban@yahoo.co
// ---------------------------------------------------
// File Name   : Atom.java
// This file contains the atom class
// this class sets basic properties of requested atoms
// ====================================================

import java.io.*;
import java.util.*;

class Atom
{
public int  number;          // atomic number
public String name;          // name of the the atom
public String symbol;        // symbol of the atom
public double mass;          // mass of the atom
public double N;             // number of the atoms
public int s[]=new int[8];
public int d[]=new int[8];
public int p[]=new int[8];
public int f[]=new int[8];
String atom_name[];
String atom_symbol[];
int oxidation_state[]=new int[7];
public Atom()
{
//empty constructor
number=0;
symbol="";
name="";
mass=0;
N=1;
}

public Atom(String st1, double NN)
{ getAtom(st1,NN); }

public Atom(String st1, int NN)
{ getAtom(st1,(double)NN); }

public Atom(String st1)
```

```
{ getAtom(st1,1.0); }

public Atom(Atom  a)
{ assign(a); }

public Atom(Atom  a, double NN)
{ assign(a); N=NN; }

//=================================================================

public void getAtom(String st1,double NN)
{
// this constructor will load Atom data from a given atom name
// or atom symbol and number of atoms
// type
String atom_name1[]={"Hydrogen", "Helium", "Lithium", "Berylium", "Boron", "Carbon", "Nitrogen", "Oxygen", "Florine",
 "Neon", "Sodium", "Magnesium", "Aliminium", "Silicon", "Phosphourus", "Sulphur", "Chlorine", "Argon", "Potassium",
 "Calcium", "Scandium", "Titanium", "Vanadium", "Chromium", "Manganese", "Iron", "Cobalt", "Nickel", "Copper", "Zinc",
 "Gallium", "Germanium", "Arsenic", "Selenium", "Bromine", "Kyrpton", "Rubidium", "Strontium","Yttirum", "Zirconium",
 "Niobium", "Molybdenium", "Technetium", "Ruthenium", "Rhodium", "Palladium", "Silver", "Cadmium", "Indium", "Tin",
 "Anthimony", "Tellerium", "Iodine", "Xenon", "Cesium", "Barium", "Lanthanum", "Cerium", "Praseodymium", "Neodymium",
 "Promethium", "Samarium", "Europium", "Gadolinium", "Terbium", "Dysprosium", "Holmium", "Erbium", "Thulium", "Ytterbium",
 "Lutetium", "Hafnium", "Tantalum", "Tungsten", "Rhenium", "Osmium", "Iridium", "Platinium", "Gold", "Mercury", "Thallium",
 "Lead", "Bismuth", "Polonium", "Astatine", "Radon", "Francium", "Radium", "Actinium", "Thorium","Protactinium","Uranium",
 "Neptunium","Plutonium","Americium","Curium","Berkelium","Californium","Einsteinium","Fermium","Mendelevium","Nobelium",
 "Lawrencium","Rutherfordium","Dubnium","Seaborgium","Bohrium","Hassium","Meithnerium","Darmstadtium","Rontgenium","Copernicium",
 "Nihonium","Flerovium","Moscovium","Livermorium","Tennesinne","Oganesson","Electron"};
atom_name=atom_name1;
String atom_symbol1[]= {"H", "He", "Li", "Be", "B", "C", "N", "O", "F", "Ne", "Na", "Mg", "Al", "Ag", "P", "S", "Cl", "Ar",
 "K", "Ca", "Se", "Ti", "V", "Cr", "Mn", "Fe", "Co", "Ni", "Cu", "Zn", "Ga", "Ge", "As", "Si", "Br", "Kr", "Ru", "Sr", "Yt",
 "Zr", "Nb", "Mo", "Tc", "Sm", "Rh", "Pd", "Ag", "Cd", "In", "Sn", "Sb","Te", "I", "Xe", "Cs", "Ba", "La", "Ce", "Pr", "Nd",
 "Pm", "Sc", "Eu", "Gd", "Tb", "Dy", "Ho", "Er", "Tm", "Yb", "Lu", "Hf", "Ta", "W", "Re", "Os", "Ir", "Pt", "Au", "Hg", "Tl",
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String atom_symbol2[]={"H", "HE", "Li", "BE", "B", "C", "N", "O", "F", "NE", "NA", "MG", "AL", "AG", "P", "S", "CL", "AR",
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 "ZR", "NB", "MO", "TC", "SM", "RH", "PD", "AG", "CD", "IN", "SN", "SB","TE", "I", "XE", "CS", "BA", "LA", "CE", "PR", "ND",
 "PM", "SC", "EU", "GD", "TB", "DY", "HO", "ER", "TM", "YB", "LU", "HF", "TA", "W", "RE", "OS", "IR", "PT", "AU", "HG", "TL",
 "PB", "Bi", "PO", "AT", "RN", "FR", "RA", "AC", "TH", "PA", "U", "NP", "PU", "AM", "CM", "BK", "CF", "ES", "FM", "MD", "NO",
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 for(int atom_number=1;atom_number<=117;atom_number++)
  {  if(st1.equals(atom_name[atom_number-1]) || st1.equals(atom_symbol1[atom_number-1]) || st1.equals(atom_symbol2[atom_number-1]) )
     {
     N=NN;
     number=atom_number;
     name=atom_name[atom_number-1];
     symbol=atom_symbol[atom_number-1];
     mass=atom_mass[atom_number-1]*N;
     break;
     }
  }
}

//=================================================================
public void assign(Atom  a)
{
number=a.number;
name=a.name;
symbol=a.symbol;
mass=a.mass;
N=a.N;
}
//=================================================================
//boolean equals logical comparisons
public boolean equals(String s)
{
boolean b;
if(name.equals(s) || symbol.equals(s))
  return true;
else
  return false;
}

public boolean equals(int n)
{
boolean b;
if(number==n)
  return true;
else
  return false;
}
//=================================================================

// this ostream function will send the symbol+number of atoms to cout
public String toString1()
{
String st=symbol;
return st;
}
```

```
public String toString()
{
String st=symbol;
if(N != 1.0)
  if(N==Math.floor(N))  st = st + (int)N;
  else                  st = st + N;
return st;
}
}

//==================================================================
```

Coefficient of the equations are given in the following table:

nam+A1:K5025e										
eqn no	a1	a2	a3	a4	a5	a6	a7	b1	b2	dhf
e-										
0	0	0	2.5	0	0	0	0	-745.375	-11.720812	0
1	0	0	2.5	0	0	0	0	-745.375	-11.720812	0
2	0	0	2.5	0	0	0	0	-745.375	-11.720812	0
Ag										
0	0	0	2.5	0	0	0	0	33520.024	6.5628194	284900
1	-330992.637	982.00864	1.3811799	6.17E-04	-1.69E-07	2.01E-11	-5.63E-16	27267.192	14.568627	284900
2	-3.72E+08	275806.92	-73.859826	0.0096062	-5.39E-07	1.36E-11	-1.27E-16	-2107725	662.83746	284900
Ag+										
0	3691132.75	-43169.83	202.84454	-0.4658414	5.59E-04	-3.15E-07	6.58E-11	337157.45	-1142.9244	1022093.7
1	-5.33E+07	131071.06	-109.88202	0.04826	-1.09E-05	1.26E-09	-5.85E-14	-743912.25	844.62662	1022093.7
2	-2.12E+08	115962.19	-22.207925	0.0029387	-1.82E-07	5.82E-12	-7.46E-17	-806801.42	227.17028	1022093.7
Ag-										
0	0	0	2.5	0	0	0	0	17665.659	5.8696798	153078.73
1	0	0	2.5	0	0	0	0	17665.659	5.8696798	153078.73
2	0	0	2.5	0	0	0	0	17665.659	5.8696798	153078.73
AL										
0	5006.60889	18.613044	2.4125311	1.99E-04	-2.43E-07	1.54E-10	-3.94E-14	38874.127	6.0865858	330000
1	-29208.20938	116.77519	2.3569065	7.74E-05	-1.53E-08	-9.97E-13	5.05E-16	38232.887	6.6009202	330000
2	-5.04E+08	380232.27	-108.23472	0.0154944	-1.07E-06	3.59E-11	-4.70E-16	-2901050.5	949.18832	330000
AL+										
0	0	0	2.5	0	0	0	0	109064.48	3.7910058	913015.13
1	-4181.18325	-9.9485573	2.5486159	-5.88E-05	3.13E-08	-7.75E-12	7.27E-16	109101.15	3.4886673	913015.13
2	-9.33E+08	567143.55	-132.08361	0.0156544	-9.32E-07	2.86E-11	-3.58E-16	-4396182.4	1177.0859	913015.13
AL-										
0	29108.00014	-383.69817	4.6551419	-0.0060458	8.58E-06	-5.48E-09	1.32E-12	34906.169	-5.9570923	281090.11
1	633982.949	-2383.4423	5.4699747	-0.0012998	2.89E-07	-3.25E-11	1.47E-15	47803.09	-15.369095	281090.11
2	5900938.3	-2295.8483	3.0727406	-6.89E-05	4.41E-09	-1.45E-13	1.91E-18	52417.489	1.4520813	281090.11
ALBO2										
0	0	0	2.3087234	0.0188905	-2.06E-05	1.03E-08	-1.69E-12	-66482.167	14.477018	-541416.21
1	0	0	7.1722995	0.0029781	-1.24E-06	2.32E-10	-1.60E-14	-67683.682	-9.9817398	-541416.21
ALBr										
0	8176.15864	-251.69427	5.4032963	-0.0017472	2.08E-06	-1.26E-09	3.17E-13	1635.0244	-2.3235949	14325.015
1	-610339.56	2010.0668	1.769618	0.0019299	-6.64E-07	1.17E-10	-7.18E-15	-12178.129	22.044508	14325.015
ALBr2										
0	31993.7587	-711.9179	9.4782581	-0.0048755	5.52E-06	-3.34E-09	8.37E-13	-15405.913	-17.421714	-140662.13
1	-352378.29	467.15442	7.1119082	-5.55E-04	3.17E-07	-5.52E-11	3.18E-15	-22650.041	-2.6956104	-140662.13
ALBr3										
0	47189.4884	-1053.8532	13.507472	-0.0066399	7.27E-06	-4.28E-09	1.05E-12	-46994.403	-36.679368	-410476.66
1	-89355.2744	-26.780351	10.02064	-8.46E-06	1.90E-09	-2.22E-13	1.04E-17	-52492.476	-15.796664	-410476.66
ALC										
0	41399.2188	-585.86779	5.9624457	-0.0020061	1.67E-06	-7.12E-10	1.27E-13	83834.361	-8.0021651	682283.51
1	1937001.487	-6749.1178	13.475256	-0.0058508	1.93E-06	-2.59E-10	1.22E-14	122536.36	-61.522449	682283.51
ALC2										
0	15240.87465	-264.99871	6.2804149	-1.79E-04	3.79E-06	-4.00E-09	1.30E-12	80927.633	-6.2472919	675615.78
1	146601.7895	-1362.7645	8.4577592	-3.68E-04	7.90E-08	-8.88E-12	4.05E-16	87059.242	-21.279567	675615.78
ALCL										
0	23808.81392	-445.71594	5.992854	-0.0027773	3.10E-06	-1.82E-09	4.41E-13	-5202.736	-7.3833052	-51007.443
1	-899346.122	2765.9421	1.0035007	0.0022678	-7.28E-07	1.18E-10	-6.66E-15	-24961.644	26.169248	-51007.443
ALCL+										
0	0	0	2.8698352	0.0066535	-1.13E-05	9.07E-09	-2.78E-12	102597.41	10.019953	861926.26
1	0	0	4.6284965	-3.48E-04	2.30E-07	-2.43E-11	-2.64E-16	102204.47	1.4303999	861926.26
ALCL2										
0	53405.4595	-967.8058	10.062527	-0.0055395	5.82E-06	-3.31E-09	7.83E-13	-26076.271	-23.933651	-240874.25
1	430345.306	-1552.3706	8.7606574	-9.47E-04	2.40E-07	-2.43E-11	8.39E-16	-21458.847	-18.036426	-240874.25
ALCL3										
0	77506.0097	-1440.7797	14.017441	-0.0063816	5.87E-06	-2.91E-09	5.99E-13	-65793.432	-44.940188	-584678.86
1	-137863.0916	-55.792073	10.041904	-1.68E-05	3.72E-09	-4.28E-13	1.98E-17	-73434.075	-20.451314	-584678.86
ALCL2+										
0	0	0	4.3561128	0.0126406	-2.16E-05	1.72E-08	-5.27E-12	56169.736	4.4930474	481172.86
1	0	0	7.0954577	4.65E-04	-2.08E-07	4.09E-11	-2.96E-15	55643.775	-8.5180986	481172.86
ALCL2-										

0	0	0	4.2510946	0.0119686	-2.15E-05	1.79E-08	-5.62E-12	-59513.061	7.3932618	-481171.19
1	0	0	6.7125618	3.47E-04	-1.59E-07	3.00E-11	-1.65E-15	-59954.257	-4.1363292	-481171.19
ALF										
0	30207.71686	-308.09869	3.8864131	0.0035643	-5.86E-06	4.39E-09	-1.26E-12	-31175.729	2.0325672	-264060.45
1	-711122.905	1903.0133	2.1916072	0.0014215	-4.18E-07	6.15E-11	-2.95E-15	-45407.29	16.131637	-264060.45
ALF+										
0	0	0	2.7253053	0.004812	-5.44E-06	2.74E-09	-3.59E-13	82250.468	9.7233611	692050.58
1	0	0	3.3522186	0.0013104	-1.43E-07	-4.54E-11	7.34E-15	82232.5	7.0837084	692050.58
ALFCL										
0	41047.7948	-576.96464	6.5626427	0.0041063	-7.21E-06	5.49E-09	-1.58E-12	-51148.287	-6.0412326	-436409.91
1	69706.3635	-622.44859	7.5734754	-2.24E-04	2.38E-08	4.44E-12	-5.49E-16	-51009.432	-10.911651	-436409.91
ALFCL+										
0	0	0	3.7341292	0.013889	-2.22E-05	1.69E-08	-5.01E-12	31647.755	6.6691475	276151.35
1	0	0	6.8835905	7.05E-04	-3.14E-07	6.16E-11	-4.45E-15	31005.99	-8.4821135	276151.35
ALFCL2										
0	69556.0734	-1188.8579	11.566726	4.57E-04	-3.41E-06	3.36E-09	-1.09E-12	-91620.493	-32.060659	-791395.4
1	-172036.0526	-119.33408	10.088944	-3.55E-05	7.83E-09	-8.96E-13	4.15E-17	-98041.855	-21.270476	-791395.4
ALF2										
0	29949.51991	-219.41999	3.4167488	0.0127295	-1.88E-05	1.33E-08	-3.68E-12	-76075.377	8.7596269	-631764.18
1	-214689.6245	30.968402	6.8163996	1.82E-04	-7.79E-08	1.47E-11	-8.80E-16	-78840.027	-7.9153705	-631764.18
ALF2+										
0	0	0	3.1239176	0.0145231	-2.13E-05	1.52E-08	-4.24E-12	9654.5072	7.4741764	92050.255
1	0	0	6.5925394	0.0010319	-4.57E-07	8.96E-11	-6.46E-15	8899.1943	-9.4596977	92050.255
ALF2-										
0	123336.7436	-1348.1937	8.6111697	2.25E-04	-2.42E-06	2.21E-09	-6.60E-13	-97084.384	-21.926128	-853230.69
1	-159007.1224	-206.05006	7.1552907	-6.26E-05	1.39E-08	-1.60E-12	7.46E-17	-104047.93	-11.226976	-853230.69
ALF2CL										
0	56774.1209	-886.98295	8.7527466	0.0081958	-1.38E-05	1.03E-08	-2.95E-12	-117793.68	-18.583478	-999128.15
1	-211542.2988	-195.91887	10.145769	-5.81E-05	1.28E-08	-1.47E-12	6.78E-17	-122715.31	-23.598538	-999128.15
ALF3										
0	44102.6352	-566.74957	5.8330729	0.0160354	-2.41E-05	1.71E-08	-4.75E-12	-144335	-5.4616137	-1209276.9
1	-249397.216	-291.12025	10.216629	-8.64E-05	1.91E-08	-2.18E-12	1.01E-16	-147569.43	-27.039832	-1209276.9
ALF4-										
0	231201.0037	-3235.3768	20.178655	-0.0091082	6.68E-06	-2.61E-09	4.11E-13	-221178.46	-86.772683	-1951600.8
1	-321741.161	-261.2097	13.197927	-8.01E-05	1.79E-08	-2.06E-12	9.61E-17	-238157.79	-42.316343	-1951600.8
ALH										
0	-37591.1403	508.90022	1.1280869	0.0039887	-2.15E-07	-2.18E-09	1.02E-12	26444.318	16.500219	249250.8
1	6802018.43	-21784.169	30.32713	-0.0150334	4.49E-06	-6.18E-10	3.12E-14	165830.12	-187.67664	249250.8
ALHCL										
0	35871.6976	-591.625	6.9445424	-0.0025115	6.47E-06	-5.64E-09	1.72E-12	2750.9305	-9.903753	10521.966
1	-168391.533	-886.23018	8.0623794	-9.20E-04	3.95E-07	-6.40E-11	3.58E-15	3641.5049	-18.006876	10521.966
ALHCL2										
0	118482.8615	-2054.1571	15.746965	-0.0147626	2.07E-05	-1.42E-08	3.83E-12	-34342.775	-57.61185	-351278.97
1	96080.6394	-1485.5402	11.035927	-3.96E-04	8.47E-08	-9.48E-12	4.32E-16	-36692.164	-32.368631	-351278.97
ALHF										
0	-9289.5451	133.55159	2.7724487	0.0067514	-4.13E-06	5.87E-10	2.28E-13	-23846.858	12.287526	-182614.48
1	734216.925	-3462.1641	10.397146	-0.0017507	4.62E-07	-5.39E-11	2.34E-15	-2965.2797	-37.131723	-182614.48
ALHFCL										
0	129037.3237	-2142.0999	14.854344	-0.0114033	1.56E-05	-1.07E-08	2.86E-12	-58183.031	-54.834255	-555244.52
1	40689.8713	-1502.1299	11.052141	-4.03E-04	8.65E-08	-9.70E-12	4.42E-16	-61298.881	-34.035646	-555244.52
ALHF2										
0	105018.1431	-1398.6542	9.1663348	0.0038673	-4.83E-06	3.10E-09	-8.44E-13	-86590.488	-25.572997	-765299.18
1	-4419.9473	-1612.8263	11.133361	-4.35E-04	9.34E-08	-1.05E-11	4.79E-16	-86069.162	-36.763838	-765299.18
ALH2										
0	14551.82996	-215.3769	5.1443702	-0.0039652	1.34E-05	-1.22E-08	3.74E-12	33110.379	-3.6087997	276774.93
1	143291.0601	-2365.9077	9.0856672	-0.0013085	4.78E-07	-7.32E-11	4.00E-15	44859.519	-32.208143	276774.93
ALH2CL										
0	93038.2898	-1328.188	9.4247636	-0.0032777	1.00E-05	-8.95E-09	2.71E-12	-7647.4379	-26.825129	-106345.41
1	316692.993	-3094.0379	12.15872	-8.25E-04	1.77E-07	-1.98E-11	9.01E-16	2411.8456	-47.183916	-106345.41
ALH2F										
0	89060.3929	-975.08039	5.8707723	0.0068967	-4.05E-06	7.22E-10	7.33E-14	-34253.026	-9.3875391	-316655.85
1	271151.4962	-3169.6235	12.214011	-8.47E-04	1.81E-07	-2.03E-11	9.25E-16	-22592.177	-49.413373	-316655.85
ALH3										
0	14812.07909	-28.364953	2.5075971	0.0073159	2.33E-06	-6.39E-09	2.46E-12	14631.894	8.3131877	128896.08
1	588545.855	-4595.7857	13.208933	-0.0012268	2.63E-07	-2.94E-11	1.34E-15	39917.17	-61.818293	128896.08
ALI										
0	1870.854131	-154.3184	5.0743919	-0.0011206	1.39E-06	-8.54E-10	2.18E-13	7517.4437	0.6688268	67395.017
1	475281.792	-1198.0286	5.4336854	-1.00E-04	-1.01E-07	4.57E-11	-3.96E-15	14646.278	-3.1411997	67395.017
ALI2										
0	14234.13595	-464.65757	8.7226749	-0.0035605	4.19E-06	-2.62E-09	6.72E-13	-3846.1333	-10.730766	-33812.954
1	-335599.902	474.33479	7.1065014	-5.53E-04	3.16E-07	-5.52E-11	3.17E-15	-9785.4889	-0.5602276	-33812.954
ALI3										
0	27060.32439	-755.99368	12.713963	-0.0054669	6.30E-06	-3.86E-09	9.77E-13	-22209.669	-28.478839	-191330.43
1	-63574.2747	-15.787723	10.012497	-5.23E-06	1.20E-09	-1.41E-13	6.67E-18	-26114.555	-12.479998	-191330.43
ALN										
0	27166.45079	-254.34911	3.5389877	0.0052963	-9.85E-06	8.45E-09	-2.59E-12	53099.949	5.3994367	438829.01
1	3821214.22	-10677.766	14.491742	-0.0037272	7.92E-07	-8.09E-11	2.89E-15	120523.63	-72.88585	438829.01
ALO										
0	-7683.3911	295.79695	0.4808108	0.0116922	-1.60E-05	1.06E-08	-2.65E-12	5843.6722	21.609978	67319.006
1	15657.21161	3855.741	-5.9260798	0.009051	-2.93E-06	4.24E-10	-2.28E-14	-13316.947	68.306634	67319.006
2	4.17E+07	-37686.088	15.47868	-9.57E-04	2.49E-08	6.69E-14	-9.00E-18	295778.65	-94.277158	67319.006
ALO+										

0	0	0	2.9414434	0.0052592	-7.34E-06	5.33E-09	-1.58E-12	118374.69	9.7353825	993004.8
1	0	0	4.1908467	6.94E-04	-3.45E-07	7.62E-11	-5.90E-15	118074.39	3.5295198	993004.8
ALO-										
0	20780.75267	2.8593512	1.9019124	0.007301	-9.14E-06	5.65E-09	-1.40E-12	-33592.677	12.963399	-272921.78
1	-69719.4829	-232.0553	4.6727843	-4.27E-05	1.63E-08	-1.73E-12	8.14E-17	-33077.189	-2.1559226	-272921.78
ALOCL										
0	-5144.62779	-58.862971	4.4523169	0.0092882	-1.25E-05	8.18E-09	-2.13E-12	-37596.837	2.4768571	-301564.57
1	-125802.7706	-242.0566	7.68113	-7.27E-05	1.61E-08	1.85E-12	8.61E-17	-37543.261	-14.758189	-301564.57
ALOCL2										
0	69026.3713	-1189.2975	11.618427	2.82E-04	-3.15E-06	3.17E-09	-1.03E-12	-44833.231	-31.654759	-402308.67
1	-170771.3922	-118.00138	10.087985	-3.51E-05	7.75E-09	-8.87E-13	4.10E-17	-51249.441	-20.592538	-402308.67
ALOF										
0	7030.57836	-115.45754	3.3788236	0.0128393	-1.75E-05	1.16E-08	-3.06E-12	-69593.817	5.9948046	-572289.6
1	-164102.0297	-327.77703	7.7445197	-9.79E-05	2.17E-08	-2.49E-12	1.15E-16	-69740.851	-17.172537	-572289.6
ALOF2										
0	47560.8529	-612.43184	6.0502237	0.0155929	-2.37E-05	1.69E-08	-4.69E-12	-91718.275	-4.9562582	-773649.77
1	-249668.1413	-283.78215	10.211081	-8.42E-05	1.86E-08	-2.12E-12	9.82E-17	-95218.042	-25.225348	-773649.77
ALOF2-										
0	0	0	2.9197597	0.024094	-3.61E-05	2.61E-08	-7.38E-12	-159181.52	11.831082	-1309625.4
1	0	0	8.6142786	0.0015785	-7.00E-07	1.37E-10	-9.90E-15	-160403.36	-15.879251	-1309625.4
ALOH										
0	58762.8383	-944.91342	7.8204459	5.86E-04	-4.08E-06	4.59E-09	-1.56E-12	-19932.97	-20.649579	-192762.17
1	788200.721	-2263.6558	7.823939	1.82E-04	-8.26E-08	1.27E-11	-6.88E-16	-10398.184	-22.090209	-192762.17
ALOH+										
0	0	0	1.9603439	0.0079191	-2.29E-06	-4.01E-09	2.57E-12	64510.185	14.106178	543933.04
1	0	0	4.1501987	0.0028925	-1.06E-06	1.79E-10	-1.16E-14	63892.888	2.6401381	543933.04
ALOH-										
0	0	0	2.9130204	0.0059531	-3.06E-06	-1.26E-09	1.29E-12	-28781.827	10.622467	-230125.63
1	0	0	4.3010718	0.0021669	-7.40E-07	1.18E-10	-7.22E-15	-29134.095	3.5270075	-230125.63
ALOHCL										
0	16363.60341	-191.59594	4.7111705	0.0138807	-2.00E-05	1.44E-08	-4.03E-12	-45680.837	4.6442018	-373785.74
1	796711.551	-2843.4705	10.9556	-1.10E-04	-1.34E-08	4.42E-12	-2.97E-16	-29698.615	-32.961146	-373785.74
ALOHCL2										
0	39719.2906	-775.15538	9.4940509	0.010744	-1.68E-05	1.26E-08	-3.61E-12	-85847.97	-19.934821	-725145.41
1	738591.539	-2863.2007	13.97062	-1.16E-04	-1.21E-08	4.26E-12	-2.90E-16	-72930.503	-46.818332	-725145.41
ALOHF										
0	-1556.003336	288.6582	0.7703793	0.0245041	-3.42E-05	2.39E-08	-6.57E-12	-71772.226	24.530718	-574211.58
1	755711.313	-2936.7028	11.024551	-1.37E-04	-7.43E-09	3.73E-12	-2.66E-16	-53401.309	-35.273973	-574211.58
ALOHF2										
0	17382.63538	-130.76873	3.3123819	0.0278473	-3.98E-05	2.81E-08	-7.76E-12	-138413.36	10.047399	-1141510.7
1	653011.992	-3034.0172	14.097198	-1.66E-04	-1.01E-09	2.99E-12	-2.32E-16	-122305.22	-51.512107	-1141510.7
ALO2										
0	43383.4649	-473.51043	6.0016157	0.0070947	-1.13E-05	8.25E-09	-2.33E-12	-3824.9859	-4.8294529	-38647.476
1	118709.0135	-833.52992	8.3092687	-3.54E-04	5.97E-08	4.07E-14	-3.52E-16	-2032.0696	-17.150402	-38647.476
ALO2-										
0	117872.2617	-1507.2349	9.5249667	-5.21E-04	-1.59E-06	1.70E-09	-5.30E-13	-48253.201	-30.813408	-452561.86
1	-187256.3912	-233.84681	7.676033	-7.09E-05	1.58E-08	-1.82E-12	8.45E-17	-55945.41	-17.737245	-452561.86
AL(OH)2										
0	4397.31691	132.76803	1.093947	0.0305406	-4.38E-05	3.17E-08	-9.00E-12	-63154.374	21.019777	-507660.67
1	1669643.735	-5924.7383	15.494803	-5.38E-04	5.41E-08	-1.20E-12	-1.08E-16	-26975.251	-66.179115	-507660.67
AL(OH)2CL										
0	24778.79709	-445.45772	5.9284702	0.0273016	-4.04E-05	2.97E-08	-8.48E-12	-103377.8	-3.6799454	-859056.72
1	1603911.487	-5767.2322	18.177723	-3.69E-04	1.14E-08	4.08E-12	-3.64E-16	-71186.999	-77.575422	-859056.72
AL(OH)2F										
0	21328.12662	-193.29002	3.0691747	0.0355502	-5.18E-05	3.75E-08	-1.06E-11	-129579.8	10.01897	-1069628.7
1	1559238.236	-5841.273	18.232299	-3.91E-04	1.61E-08	3.54E-12	-3.39E-16	-96231.009	-79.713518	-1069628.7
AL(OH)3										
0	-14024.75452	369.60735	-0.2979601	0.0492986	-6.98E-05	5.01E-08	-1.41E-11	-125526.08	27.114901	-1012667.5
1	2477063.616	-8968.6173	22.80321	-8.32E-04	8.66E-08	-2.42E-12	-1.33E-16	-70152.786	-112.18992	-1012667.5
ALS										
0	26117.42801	-347.06739	4.4362046	0.0033402	-8.41E-06	8.51E-09	-2.78E-12	28637.791	0.752296	232682.01
1	8909844.29	-25076.775	28.934561	-0.0098398	2.05E-06	-2.09E-10	8.15E-15	188576.16	-178.60362	232682.01
ALS2										
0	42523.3541	-776.46033	9.801069	-0.0039107	3.88E-06	-2.08E-09	4.68E-13	31679.615	-21.780946	248535.28
1	-68525.6354	-26.716677	7.5201939	-8.15E-06	1.81E-09	-2.09E-13	9.70E-18	27583.627	-7.8734573	248535.28
AL2										
0	-5281.50965	-17.273745	4.604077	-2.62E-04	6.30E-07	-3.29E-10	8.89E-14	59007.064	3.0601889	501301.72
1	-2320724.102	9218.7079	-9.4469519	0.0099999	-3.15E-06	4.36E-10	-2.24E-14	2904.5895	99.603207	501301.72
AL2Br6										
0	64833.197	-1947.6878	28.869898	-0.0136583	1.56E-05	-9.49E-09	2.39E-12	-110152.68	-102.59348	-942422.81
1	-173182.949	-43.422998	22.034142	-1.42E-05	3.24E-09	-3.80E-13	1.80E-17	-120233.84	-62.01055	-942422.81
AL2C2										
0	11109.87147	-350.24342	8.598856	0.0018325	1.04E-06	-2.09E-09	7.72E-13	64927.642	-16.450802	544978
1	159765.1967	-1644.0072	11.646437	-4.38E-04	9.37E-08	-1.05E-11	4.78E-16	72048.898	-36.481643	544978
AL2CL6										
0	134093.5279	-3001.038	31.430009	-0.0170041	1.79E-05	-1.02E-08	2.41E-12	-147183	-127.44454	-1296876.2
1	-275297.5554	-92.48236	22.070582	-2.87E-05	6.42E-09	-7.44E-13	3.47E-17	-162915.7	-70.916031	-1296876.2
AL2F6										
0	191506.1289	-3168.2403	22.453748	0.0127153	-2.49E-05	1.96E-08	-5.71E-12	-304996.26	-93.964731	-2632491.2
1	-585298.261	-545.0572	22.406863	-1.63E-04	3.60E-08	-4.12E-12	1.91E-16	-321968.39	-85.898679	-2632491.2
AL2I6										
0	25875.71514	-1280.7197	26.777158	-0.009913	1.17E-05	-7.30E-09	1.87E-12	-58911.056	-83.302093	-487747.04

1	-121011.2399	-24.675428	22.019927	-8.46E-06	1.96E-09	-2.33E-13	1.11E-17	-65485.238	-55.285365	-487747.04
AL2O										
0	7776.5307	-129.42354	4.9125095	0.0086042	-1.22E-05	8.31E-09	-2.24E-12	-18865.129	-0.0280637	-148611.29
1	-117107.4351	-178.30092	7.6332154	-5.34E-05	1.18E-08	-1.36E-12	6.29E-17	-19475.801	-14.157642	-148611.29
AL2O+										
0	0	0	4.1045736	0.0119784	-1.85E-05	1.38E-08	-3.99E-12	76852.703	5.1025724	652444.09
1	0	0	6.8797855	7.07E-04	-3.14E-07	6.16E-11	-4.45E-15	76270.756	-8.3318145	652444.09
AL2O2										
0	-19405.60042	250.84898	3.6214038	0.0195139	-2.56E-05	1.66E-08	-4.31E-12	-51726.973	9.9239959	-403095.59
1	-194061.1656	-460.97524	10.843756	-1.38E-04	3.04E-08	-3.50E-12	1.62E-16	-49630.558	-29.465381	-403095.59
AL2O2+										
0	0	0	3.3421904	0.0281112	-4.95E-05	4.05E-08	-1.26E-11	66362.506	9.2902416	567422.01
1	0	0	9.2751693	8.36E-04	-3.74E-07	7.36E-11	-5.33E-15	65264.068	-18.677259	567422.01
AL2O3										
0	-7443.37432	88.290042	5.2646626	0.0250768	-3.43E-05	2.30E-08	-6.12E-12	-68726.86	2.2023243	-546890.53
1	-277778.4969	-491.74659	13.867039	-1.47E-04	3.25E-08	-3.73E-12	1.73E-16	-67907.579	-43.755599	-546890.53
AL2S										
0	40946.2437	-779.71725	9.8144231	-0.0039403	3.91E-06	-2.11E-09	4.75E-13	28339.633	-24.650658	220679.13
1	-70434.3737	-26.763769	7.5202338	-8.17E-06	1.82E-09	-2.09E-13	9.73E-18	24227.184	-10.665792	220679.13
AL2S2										
0	66145.8732	-1111.3195	12.570073	-0.0014561	-5.85E-07	1.39E-09	-5.50E-13	19144.569	-36.002746	135287.32
1	-137780.6456	-77.050325	10.557236	-2.28E-05	5.01E-09	-5.72E-13	2.64E-17	13133.361	-22.568491	135287.32
Ar										
0	0	0	2.5	0	0	0	0	-745.375	4.3796749	0
1	20.10538475	-0.0599266	2.5000694	-3.99E-08	1.21E-11	-1.82E-15	1.08E-19	-744.99396	4.3791801	0
2	-9.95E+08	645888.73	-167.58947	0.0231993	-1.72E-06	6.53E-11	-9.74E-16	-5078300.3	1465.2985	0
Ar+										
0	-57312.0917	793.07915	-1.7171212	0.0104418	-1.18E-05	6.53E-09	-1.45E-12	179057.22	29.49151	1526778.4
1	-383596.54	816.20197	2.3013426	-4.95E-06	1.21E-08	-2.19E-12	1.27E-16	177181.15	7.9475075	1526778.4
2	1.02E+07	-6685.1041	4.4609538	-3.03E-04	2.62E-08	-1.21E-12	2.30E-17	235435.35	-10.445193	1526778.4
B										
0	118.2394638	-0.0700992	2.5002362	-4.58E-07	5.12E-10	-3.06E-13	7.53E-17	68483.591	4.2095019	575598.76
1	-107265.961	322.53072	2.1264072	2.11E-04	-5.94E-08	7.38E-12	-2.28E-16	66434.131	6.8770697	575598.76
2	-4.15E+08	232957.68	-47.209137	0.0048777	-2.07E-07	3.23E-12	-1.82E-18	-1802904.7	443.96176	575598.76
B+										
0	0.078497912	-8.95E-04	2.5000041	-9.58E-09	1.22E-11	-7.99E-15	2.11E-18	164233.29	2.4190536	1371716.7
1	-8911.54803	4.5877901	2.5315001	-4.90E-05	2.85E-08	-7.38E-12	7.12E-16	164177.9	2.2386698	1371716.7
2	-7.98E+08	473404.49	-105.5286	0.0117031	-6.08E-07	1.48E-11	-1.33E-16	-3610391.7	949.73998	1371716.7
B-										
0	22.01568105	-0.0047405	2.5000142	-2.50E-08	2.56E-11	-1.42E-14	3.27E-18	63243.183	4.6163673	532032.7
1	21.18018248	2.07E-04	2.4999997	1.46E-10	-3.89E-14	5.09E-18	-2.60E-22	63243.156	4.6164558	532032.7
2	-131.1386485	0.0902891	2.4999786	2.61E-09	-1.72E-13	5.81E-18	-7.93E-23	63242.439	4.6166403	532032.7
BBr										
0	37960.935	-497.6096	5.2670082	-3.74E-05	-1.13E-06	1.26E-09	-4.29E-13	30381.254	-4.3534073	240952.36
1	253685.8027	-640.59095	4.6668235	4.18E-04	-2.96E-07	7.52E-11	-4.84E-15	31890.843	-0.8255871	240952.36
BBr2										
0	65165.5071	-902.95908	8.0638178	0.0011298	-4.20E-06	3.97E-09	-1.28E-12	14704.664	-13.364532	97828.617
1	-419163.337	415.76885	7.1481698	-5.69E-04	3.20E-07	-5.55E-11	3.19E-15	6118.9821	-5.5027596	97828.617
BBr3										
0	39680.7369	-633.10872	8.0545516	0.0097776	-1.61E-05	1.22E-08	-3.52E-12	-23667.233	-11.060994	-205300
1	-190104.6795	-150.36277	10.109999	-4.32E-05	9.41E-09	-1.07E-12	4.88E-17	-27425.531	-19.97496	-205300
BC										
0	-39157.58	728.45381	-1.5527434	0.015529	-1.98E-05	1.27E-08	-3.23E-12	96449.137	32.482045	838161.91
1	-2346280.674	6450.7513	-2.6195324	0.0033392	-4.51E-07	1.35E-11	8.27E-16	57866.851	50.378849	838161.91
BC2										
0	-29874.22175	364.31266	2.9634694	0.0065618	-3.54E-06	1.93E-10	3.12E-13	93048.357	10.834242	801258.73
1	1525485.889	-5987.8624	14.083849	-0.0037475	1.08E-06	-1.38E-10	6.47E-15	131120.4	-63.372155	801258.73
BCL										
0	22024.58989	-170.05112	3.0660759	0.0055951	-8.46E-06	6.08E-09	-1.70E-12	21974.025	6.3889692	183173.44
1	-74212.6254	263.80901	3.6002277	0.0010189	-4.67E-07	9.85E-11	-6.47E-15	19127.265	5.2353082	183173.44
BCL+										
0	0	0	2.8124197	0.0046006	-4.81E-06	1.97E-09	-1.38E-13	147448.49	9.1566825	1234312.3
1	0	0	4.1060888	4.73E-04	-1.79E-07	3.24E-11	-2.05E-15	147130.97	2.6427295	1234312.3
BCLOH										
0	-28984.27288	689.40466	-2.2881381	0.0334943	-4.73E-05	3.33E-08	-9.22E-12	-32619.811	39.768859	-234005.38
1	702773.844	-2857.3913	10.911758	-8.11E-05	-2.12E-08	5.41E-12	-3.46E-16	-13072.219	-35.851695	-234005.38
BCL(OH)2										
0	80726.2301	-859.46198	2.7050396	0.038788	-5.72E-05	4.15E-08	-1.17E-11	-93799.107	7.1349771	-805387.66
1	1423878.191	-5849.7041	17.921652	-2.01E-04	-3.39E-08	9.84E-12	-6.47E-16	-64742.618	-81.004001	-805387.66
BCL2										
0	35988.7942	-360.28265	4.1576855	0.0115288	-1.82E-05	1.34E-08	-3.84E-12	-6765.1071	5.1823009	-60881.49
1	350140.313	-1662.2036	8.8395347	-9.77E-04	2.47E-07	-2.50E-11	8.72E-16	568.29094	-21.483494	-60881.49
BCL2+										
0	0	0	4.2704931	0.0106038	-1.42E-05	8.54E-09	-1.83E-12	79436.016	4.0764507	674064.43
1	0	0	6.9266627	6.78E-04	-3.21E-07	6.83E-11	-5.01E-15	78857.822	-8.9346266	674064.43
BCL2-										
0	0	0	3.2358791	0.0116902	-1.48E-05	8.22E-09	-1.57E-12	-18981.815	10.69001	-146439.37
1	0	0	6.3518218	7.70E-04	-4.47E-07	1.38E-10	-1.32E-14	-19705.432	-4.7747207	-146439.37
BCL2OH										
0	20997.5517	-247.06992	2.5787617	0.0312036	-4.55E-05	3.24E-08	-9.04E-12	-73090.286	12.736577	-604917.44
1	587811.379	-2982.9693	14.00662	-1.19E-04	-1.27E-08	4.42E-12	-3.00E-16	-58241.681	-51.508591	-604917.44
BCL3										

0	23929.70339	-414.03789	5.4880353	0.016484	-2.46E-05	1.74E-08	-4.85E-12	-48394.698	-1.6753667	-404500
1	-241740.8819	-292.15395	10.216685	-8.62E-05	1.90E-08	-2.17E-12	1.00E-16	-50748.344	-25.468635	-404500
BF										
0	-52389.5473	811.84766	-1.1416149	0.0116125	-1.18E-05	6.02E-09	-1.24E-12	-17745.42	30.050863	-106931.88
1	-374638.978	560.44939	3.6091861	6.19E-04	-1.78E-07	2.43E-11	-9.39E-16	-18191.793	3.7166093	-106931.88
BFCL										
0	-23635.12735	438.3169	0.3918096	0.0171999	-2.14E-05	1.34E-08	-3.37E-12	-36871.666	26.681021	-279184.07
1	-108630.9561	-523.34385	7.2975047	-3.05E-05	-3.15E-08	1.05E-11	-7.62E-16	-33058.912	-11.865873	-279184.07
BFCL2										
0	4402.55124	-157.13989	4.0163223	0.017434	-2.25E-05	1.43E-08	-3.65E-12	-78224.526	6.8860858	-643000
1	-223361.3309	-644.0603	10.478618	-1.91E-04	4.22E-08	-4.85E-12	2.25E-16	-77406.265	-28.146315	-643000
BFOH										
0	-75639.5367	1354.8381	-5.6482101	0.0387027	-5.04E-05	3.34E-08	-8.85E-12	-61944.461	58.003628	-451631.68
1	725131.809	-3215.6209	11.179098	-1.88E-04	2.58E-09	2.67E-12	-2.19E-16	-37168.081	-39.784635	-451631.68
BF(OH)2										
0	13818.00676	252.9637	-3.844552	0.0525514	-7.19E-05	4.95E-08	-1.35E-11	-128312.33	42.936594	-1049889.5
1	1422037.64	-6257.2976	18.224607	-3.22E-04	-7.13E-09	6.76E-12	-5.04E-16	-91862.542	-85.278951	-1049889.5
BF2										
0	-67876.5176	1085.9035	-3.023321	0.023265	-2.64E-05	1.52E-08	-3.52E-12	-66409.183	44.319683	-499426.9
1	-115309.1296	-810.98001	7.6027092	-2.41E-04	5.33E-08	-6.12E-12	2.84E-16	-57962.222	-16.55644	-499426.9
BF2+										
0	0	0	3.3146474	0.0086444	-6.75E-06	1.34E-09	4.51E-13	37483.649	5.9046898	322597.38
1	0	0	5.8127638	0.0018193	-7.71E-07	1.45E-10	-9.98E-15	36794.801	-7.0043119	322597.38
BF2-										
0	21097.65318	143.95646	0.2604646	0.0181737	-2.24E-05	1.37E-08	-3.36E-12	-89718.018	23.516926	-733802.96
1	-170992.0627	-615.62198	7.4588714	-1.84E-04	4.06E-08	-4.67E-12	2.17E-16	-87414.045	-16.206047	-733802.96
BF2CL										
0	4500.10125	-119.6285	3.1986351	0.0174343	-1.99E-05	1.13E-08	-2.54E-12	-107677.99	10.081945	-888000
1	-206681.7398	-1024.4473	10.75844	-3.02E-04	6.67E-08	-7.65E-12	3.55E-16	-104693.67	-32.299956	-888000
BF2OH										
0	-7522.52165	436.71217	-3.1289735	0.0432396	-5.79E-05	3.89E-08	-1.04E-11	-134425.95	41.391706	-1092217.3
1	576075.925	-3611.9002	14.468976	-3.03E-04	2.76E-08	-1.91E-13	-8.69E-17	-113358.9	-58.969815	-1092217.3
BF3										
0	3465.584	21.331987	1.6412452	0.0199376	-2.15E-05	1.15E-08	-2.44E-12	-137945.56	16.255335	-1136000
1	-181976.7014	-1405.3479	11.034123	-4.10E-04	9.03E-08	-1.03E-11	4.78E-16	-132313.69	-37.383861	-1136000
BF4-										
0	206848.52	-2463.1908	12.064142	0.0110277	-1.75E-05	1.20E-08	-3.15E-12	-201056.92	-46.108269	-1761266
1	-437324.171	-775.92894	13.582226	-2.34E-04	5.20E-08	-5.98E-12	2.78E-16	-212725.19	-49.533697	-1761266
BH										
0	20630.8255	-368.25025	6.0713379	-0.0087283	1.46E-05	-1.04E-08	2.78E-12	55566.291	-13.003926	456723.2
1	-1098531.663	-174.58901	8.4424268	-0.0054402	2.72E-06	-4.84E-10	2.87E-14	51129.049	-29.710307	456723.2
2	1.67E+07	-47392.393	30.026195	-0.0040667	2.73E-07	-8.93E-12	1.16E-16	377229.78	-214.27125	456723.2
BHCL										
0	47632.7491	-442.00165	3.9756459	0.0085417	-1.38E-05	1.13E-08	-3.57E-12	18222.784	3.0284429	141418.31
1	349999.172	-2238.4048	8.7111061	-0.0010889	4.19E-07	-6.57E-11	3.62E-15	28412.404	-25.895672	141418.31
BHCL2										
0	44199.1481	-238.47396	1.3566822	0.0251787	-3.63E-05	2.64E-08	-7.63E-12	-30038.779	17.870235	-251883.53
1	411099.606	-2858.0274	11.795475	-6.32E-04	1.27E-07	-1.35E-11	5.92E-16	-16172.888	-42.179021	-251883.53
BHF										
0	-49083.6226	961.07602	-2.9198503	0.0214916	-2.60E-05	1.69E-08	-4.55E-12	-14669.252	41.607093	-76012.343
1	1184821.3	-4677.4352	10.673281	-0.0016064	3.70E-07	-3.80E-11	1.43E-15	18026.409	-42.859312	-76012.343
BHFCL										
0	576.116972	304.21563	-0.98089	0.0280384	-3.68E-05	2.50E-08	-6.87E-12	-60502.074	31.328414	-483036.62
1	439077.892	-3137.1817	12.002862	-7.15E-04	1.45E-07	-1.57E-11	6.91E-16	-42323.683	-44.665436	-483036.62
BHF2										
0	-83535.4028	1616.6598	-8.1614057	0.0415379	-4.92E-05	3.05E-08	-7.79E-12	-97480.655	70.386308	-739613.81
1	466087.696	-3728.1005	12.441527	-8.91E-04	1.84E-07	-2.01E-11	8.98E-16	-69781.429	-51.03218	-739613.81
BH2										
0	37527.9773	-487.73331	6.3401728	-0.0061367	1.19E-05	-7.12E-09	1.31E-12	39476.687	-12.908415	318289.28
1	1565810.423	-6858.1843	13.297596	-0.002706	6.14E-07	-7.10E-11	3.29E-15	78599.654	-66.384302	318289.28
BH2CL										
0	16466.38117	127.73209	0.1300269	0.0193814	-2.32E-05	1.61E-08	-4.67E-12	-11121.122	23.084992	-80845.754
1	1427215.437	-6265.5643	13.82183	-0.0013138	2.59E-07	-2.71E-11	1.17E-15	26393.875	-63.997262	-80845.754
BH2F										
0	-88379.2044	1705.2859	-8.0612461	0.0364319	-4.15E-05	2.62E-08	-6.93E-12	-47872.734	68.620877	-323956.73
1	1435082.111	-6625.3202	14.09165	-0.0014225	2.83E-07	-2.99E-11	1.30E-15	-793.71927	-68.013564	-323956.73
BH3										
0	-44307.912	679.22573	0.469892	0.0057022	4.14E-06	-5.58E-09	1.68E-12	6145.4248	20.087138	88000
1	2431957.621	-9585.5476	15.871438	-0.0020267	4.01E-07	-4.22E-11	1.83E-15	68190.15	-87.15538	88000
BH3NH3										
0	-181106.3598	3010.3415	-15.242711	0.0621564	-5.96E-05	3.27E-08	-7.75E-12	-29342.789	108.73996	-115000
1	4354925.96	-18242.352	31.629998	-0.0032082	5.89E-07	-5.81E-11	2.38E-15	94381.18	-189.78658	-115000
BI										
0	35174.4953	-544.58193	6.027511	-0.0023872	2.24E-06	-1.11E-09	2.28E-13	40719.101	-7.2880498	325987.5
1	2132872.626	-6283.685	11.239643	-0.0032589	7.06E-07	-4.23E-11	-4.21E-16	77976.348	-46.640426	325987.5
BI2										
0	66409.759	-1044.412	9.7341972	-0.0039526	3.17E-06	-1.27E-09	1.88E-13	32057.509	-20.124071	238096.32
1	-392402.223	442.29024	7.1296236	-5.62E-04	3.18E-07	-5.54E-11	3.18E-15	22919.726	-3.2017932	238096.32
BI3										
0	62431.1489	-1002.4086	11.066501	0.0016096	-5.15E-06	4.73E-09	-1.51E-12	5160.3482	-24.206876	21400
1	-150617.6506	-81.672106	10.059379	-2.32E-05	5.02E-09	-5.65E-13	2.58E-17	-426.16879	-16.179628	21400
BN										

0	-45697.0758	670.42861	0.0361509	0.0073395	-4.97E-06	1.23E-09	6.34E-14	64854.651	25.398701	574726.41
1	-227693.2705	-102.56493	4.4145868	2.56E-04	-1.61E-08	-6.53E-13	5.75E-17	67844.651	-0.6778544	574726.41
BO										
0	-11662.16822	92.175794	3.6554985	-0.0031185	9.01E-06	-8.02E-09	2.47E-12	873.82848	4.4828474	20406.404
1	17886.00589	-630.90196	4.5745284	1.99E-04	-9.70E-08	1.87E-11	-1.03E-15	4841.3111	-3.3988906	20406.404
2	-1.59E+08	121095.56	-31.368235	0.00511	-3.46E-07	1.15E-11	-1.50E-16	-934506.58	302.61239	20406.404
BO-										
0	-82420.2321	920.36369	-0.230266	0.0062299	-3.16E-06	1.18E-10	2.82E-13	-39111.412	25.992268	-277791.08
1	212280.4369	-1262.1247	5.3831673	-3.18E-04	7.29E-08	-8.14E-12	3.72E-16	-27068.923	-9.7737537	-277791.08
BOCL										
0	70523.8064	-1315.3014	11.300877	-0.0120711	1.88E-05	-1.37E-08	3.85E-12	-33553.991	-36.984632	-318536.7
1	155714.8487	-1446.255	8.5094481	-3.86E-04	8.26E-08	-9.26E-12	4.22E-16	-32035.89	-23.72714	-318536.7
BOCL2										
0	7322.66736	-202.7727	4.1619241	0.0173331	-2.26E-05	1.45E-08	-3.72E-12	-44144.419	6.5204149	-361565.51
1	-229752.7041	-619.45679	10.460755	-1.84E-04	4.07E-08	-4.67E-12	2.17E-16	-43715.384	-27.435711	-361565.51
BOF										
0	72268.0265	-1131.3866	8.8160545	-0.0046277	7.80E-06	-5.68E-09	1.53E-12	-67111.16	-25.479572	-592978.31
1	193702.0297	-1739.1123	8.6956509	-4.52E-04	9.59E-08	-1.07E-11	4.84E-16	-63301.524	-27.024586	-592978.31
BOF2										
0	7227.79413	21.487836	1.1578403	0.0225059	-2.61E-05	1.51E-08	-3.52E-12	-101399.57	20.101271	-832767.7
1	-220502.8861	-1254.2387	10.925514	-3.68E-04	8.11E-08	-9.28E-12	4.30E-16	-96804.476	-34.828533	-832767.7
BOH										
0	-75214.1027	1391.4447	-5.6303302	0.0296636	-3.83E-05	2.55E-08	-6.80E-12	-8341.3003	55.1769	-6756.578
1	844749.857	-3016.9829	8.0838647	-1.61E-04	-2.19E-09	3.13E-12	-2.38E-16	16476.985	-26.032279	-6756.578
BO2										
0	-41410.9064	719.88546	-1.4776294	0.0227742	-2.79E-05	1.72E-08	-4.28E-12	-41776.577	32.58458	-309121.95
1	-38344.5234	-956.32611	8.2009628	-2.06E-04	9.87E-09	8.16E-12	-7.53E-16	-34235.64	-22.247723	-309121.95
BO2-										
0	53242.7969	-732.6313	5.90247	0.0024375	-4.88E-07	-8.48E-10	4.08E-13	-83442.937	-10.539319	-714493.99
1	119922.6372	-1715.767	8.7010382	-4.60E-04	9.87E-08	-1.11E-11	5.05E-16	-78257.897	-28.393565	-714493.99
B(OH)2										
0	1491.659222	364.81848	-2.9060064	0.0413683	-5.78E-05	4.07E-08	-1.13E-11	-53754.837	38.885352	-425243.64
1	1557023.406	-5784.7108	14.873912	-1.82E-04	-3.80E-08	1.03E-11	-6.69E-16	-18068.103	-65.902689	-425243.64
BS										
0	-38394.901	698.94175	-1.2139805	0.0139639	-1.69E-05	1.04E-08	-2.58E-12	28656.855	31.548234	273519.41
1	1358760.165	-4364.036	9.0343076	-0.0021145	4.19E-07	-1.35E-11	-1.36E-15	59130.655	-33.366934	273519.41
BS2										
0	18202.64374	-515.06719	8.547515	-0.0016262	1.87E-06	-1.28E-09	3.68E-13	8186.8398	-17.783809	63867.46
1	512040.251	-1938.5811	9.8148735	-0.0013397	3.75E-07	-4.40E-11	1.89E-15	17365.35	-27.575427	63867.46
B2										
0	-151641.8096	2630.1689	-13.813583	0.0521623	-6.93E-05	4.47E-08	-1.13E-11	89952.511	98.131185	857370.51
1	1094594.495	-2602.7357	6.9094562	-6.41E-04	1.95E-07	-2.56E-11	1.05E-15	118780.76	-19.49045	857370.51
B2C										
0	-41665.1987	579.77795	1.4110171	0.0117471	-1.07E-05	4.72E-09	-7.97E-13	91968.742	17.692544	800432.61
1	1159241.019	-4567.7988	12.286721	-0.0025008	6.41E-07	-6.93E-11	2.67E-15	122244.21	-51.990662	800432.61
B2CL4										
0	42855.5513	-728.07488	9.3157637	0.0233163	-3.51E-05	2.46E-08	-6.74E-12	-58190.232	-16.22085	-490000
1	-642798.703	507.8563	14.86725	2.03E-06	6.27E-09	-1.22E-12	7.24E-17	-68200.66	-41.391118	-490000
B2F4										
0	-59716.9564	818.94254	-0.6437671	0.0385897	-4.31E-05	2.40E-08	-5.39E-12	-179004.12	35.5218	-1438000
1	38558.6589	-2928.8427	17.920637	-9.52E-04	1.61E-07	-1.43E-11	5.22E-16	-161305.19	-71.848033	-1438000
B2H6										
0	19268.58874	558.28525	-6.2177136	0.0484741	-4.52E-05	2.52E-08	-6.45E-12	1337.4273	52.715581	36600
1	2852173.433	-15632.597	32.224186	-0.0037226	7.68E-07	-8.37E-11	3.73E-15	93384.116	-191.56873	36600
B2O										
0	-56995.4676	1018.0005	-2.6364819	0.0274601	-3.63E-05	2.41E-08	-6.38E-12	17038.744	38.553461	192798.02
1	-162872.322	-387.62898	7.7877235	-1.15E-04	2.53E-08	-2.89E-12	1.34E-16	22630.354	-19.08513	192798.02
B2O2										
0	81743.9169	-1732.7028	16.055609	-0.0216006	3.57E-05	-2.66E-08	7.53E-12	-48996.329	-61.727024	-457711.49
1	460578.966	-2990.0792	12.567641	-7.85E-04	1.67E-07	-1.87E-11	8.49E-16	-40157.482	-48.744137	-457711.49
B2O3										
0	73796.1191	-1263.6206	10.726815	3.84E-04	5.98E-06	-6.55E-09	2.12E-12	-96281.831	-30.88078	-835382.27
1	390503.53	-3691.3482	15.555026	-9.71E-04	2.07E-07	-2.31E-11	1.05E-15	-82630.544	-63.908634	-835382.27
B2(OH)4										
0	-17287.17249	849.59135	-8.7159596	0.0936236	-1.28E-04	8.81E-08	-2.40E-11	-156433.71	71.201693	-1254987.5
1	2983925.656	-12074.696	31.626106	-5.16E-04	-4.23E-08	1.67E-11	-1.16E-15	-82809.77	-165.30105	-1254987.5
B2S										
0	66386.093	-920.11857	8.6998313	7.65E-04	-3.71E-06	3.64E-09	-1.20E-12	77703.758	-22.517097	622260.71
1	-121150.1483	-64.733985	7.5468256	-1.82E-05	3.92E-09	-4.40E-13	2.00E-17	72585.319	-13.949684	622260.71
B2S2										
0	-70615.4997	718.29448	1.9197978	0.0203641	-2.31E-05	1.31E-08	-3.00E-12	11008.29	18.554061	138317.11
1	-164153.5014	-774.28656	11.077317	-2.31E-04	5.13E-08	-5.89E-12	2.74E-16	17330.035	-33.597635	138317.11
B2S3										
0	-34312.685	558.76154	3.4140774	0.0239833	-2.84E-05	1.69E-08	-4.06E-12	-3027.6906	18.467717	17754.057
1	-190585.5086	-934.83425	13.693336	-2.77E-04	6.11E-08	-7.01E-12	3.25E-16	2906.4338	-39.468667	17754.057
B3N3H6										
0	-155262.1082	4010.2113	-33.824913	0.1624576	-2.07E-04	1.37E-07	-3.67E-11	-80512.534	199.50008	-512000
1	3739245.17	-19412.39	44.4507	-0.0032103	5.72E-07	-5.49E-11	2.19E-15	47584.262	-264.11566	-512000
B3O3CL3										
0	-42844.528	1005.624	-4.5565196	0.0811797	-1.04E-04	6.62E-08	-1.70E-11	-204090.73	54.661131	-1635982
1	-741405.981	-2527.4475	26.872637	-7.46E-04	1.65E-07	-1.89E-11	8.74E-16	-192350.99	-118.56363	-1635982
B3O3FCL2										

0	-37191.2007	867.37459	-4.0957785	0.0781556	-9.77E-05	6.10E-08	-1.53E-11	-233138.36	51.980876	-1883807.7
1	-716236.083	-2851.2103	27.109531	-8.40E-04	1.85E-07	-2.12E-11	9.83E-16	-220272.93	-121.06794	-1883807.7
B3O3F2CL										
0	-52770.1554	1104.9047	-5.8541811	0.0795394	-9.59E-05	5.80E-08	-1.42E-11	-264040.01	60.712469	-2132816.8
1	-681078.749	-3370.009	27.489536	-9.91E-04	2.18E-07	-2.50E-11	1.16E-15	-247211.48	-126.15016	-2132816.8
B3O3F3										
0	-72515.4978	1400.9962	-7.9067162	0.0821716	-9.63E-05	5.67E-08	-1.35E-11	-295346.17	70.015368	-2382699.1
1	-662982.291	-3784.9469	27.795266	-0.0011121	2.45E-07	-2.81E-11	1.30E-15	-274886.55	-131.5605	-2382699.1
Ba										
0	2222.563526	-34.079779	2.7067511	-6.38E-04	1.06E-06	-9.10E-10	3.15E-13	21665.497	5.1025459	185000
1	-1.93E+07	60065.01	-66.339641	0.0350757	-7.81E-06	8.09E-10	-3.20E-14	-358966.37	500.75834	185000
2	3.48E+08	-292555.83	97.748885	-0.0134548	9.57E-07	-3.38E-11	4.73E-16	2250335.3	-796.84444	185000
Ba+										
0	-54231.6755	674.46808	-0.8940273	0.0087966	-1.22E-05	8.39E-09	-2.04E-12	79417.746	26.070637	694049.53
1	8794971.85	-19518.179	14.855429	-9.40E-04	-7.03E-07	1.67E-10	-1.07E-14	214680.07	-92.282642	694049.53
2	-1.06E+08	45307.996	-0.5410673	-7.53E-04	1.30E-07	-6.01E-12	8.85E-17	-300087.47	43.706108	694049.53
BaBr										
0	-691.255744	-62.455002	4.7966777	-6.84E-04	1.04E-06	-7.44E-10	2.17E-13	-10113.492	5.1964549	-75324.677
1	-1056014.042	1034.7402	6.7357294	-0.003784	1.95E-06	-3.35E-10	1.89E-14	-19502.336	-5.0692796	-75324.677
BaBr2										
0	-5143.37406	-38.705185	7.162447	-3.70E-04	4.69E-07	-3.11E-10	8.36E-14	-51533.183	0.9741407	-412514.74
1	-8928.25121	-0.7536559	7.0006582	-2.95E-07	7.09E-11	-8.67E-15	4.22E-19	-51726.695	1.9101857	-412514.74
BaCL										
0	-2661.946867	-77.249963	4.7461061	-3.52E-04	4.00E-07	-1.94E-10	4.12E-14	-17363.281	3.9044525	-136290.88
1	-1075410.089	1209.3031	6.2725586	-0.0032881	1.72E-06	-2.91E-10	1.63E-14	-27791.737	-3.5741878	-136290.88
BaCL+										
0	-895.155669	-133.46927	4.9354161	-7.57E-04	8.36E-07	-4.69E-10	1.10E-13	41251.56	1.8962758	348697.63
1	-18291.98157	-2.9316167	4.5022807	3.67E-05	2.40E-09	5.48E-14	1.17E-18	40551.002	4.503763	348697.63
BaCL2										
0	-1157.501999	-205.45188	7.8375141	-0.0018677	2.34E-06	-1.53E-09	4.09E-13	-61156.653	-5.9781535	-499301.39
1	-22165.98768	-4.0024838	7.0034267	-1.52E-06	3.61E-10	-4.39E-14	2.13E-18	-62190.953	-1.132444	-499301.39
BaF										
0	25303.17292	-471.69951	6.1850362	-0.0033667	4.01E-06	-2.51E-09	6.48E-13	-37318.721	-6.2207154	-318993.79
1	1868380.434	-7071.0996	14.669593	-0.006996	2.37E-06	-3.29E-10	1.65E-14	3571.7807	-66.623909	-318993.79
BaF+										
0	28407.19922	-486.35718	5.9460584	-0.0024298	2.45E-06	-1.32E-09	2.97E-13	17306.391	-5.9512069	134063.21
1	-40544.2367	-17.019977	4.5130553	2.63E-05	2.61E-09	-9.50E-14	6.52E-18	14744.866	2.7831677	134063.21
BaF2										
0	34883.9552	-764.84596	9.7977504	-0.0057565	6.78E-06	-4.24E-09	1.09E-12	-95903.565	-20.820353	-812003.48
1	-55086.3366	-16.911142	7.0135649	-5.73E-06	1.32E-09	-1.57E-13	7.44E-18	-99835.297	-4.3895815	-812003.48
BaH										
0	-37652.6888	698.66801	-1.3135244	0.0146065	-1.80E-05	1.13E-08	-2.87E-12	20974.789	32.308026	209535.11
1	-6755466.57	17307.002	-11.368125	0.0056177	-3.18E-07	-1.05E-10	1.11E-14	-89540.704	118.23775	209535.11
BaI										
0	-4186.28554	10.330946	4.4289002	3.03E-04	-2.59E-07	1.74E-10	-3.37E-14	-2636.1697	8.2019247	-10237.675
1	-3533859.66	7394.258	1.2851515	-0.0023034	2.21E-06	-4.68E-10	3.01E-14	-53402.296	37.104439	-10237.675
BaI2										
0	-4241.59273	-18.622144	7.0785568	-1.79E-04	2.28E-07	-1.51E-10	4.08E-14	-36703.515	3.163139	-288439.97
1	-6048.2248	-0.3622729	7.0003175	-1.43E-07	3.43E-11	-4.20E-15	2.05E-19	-36796.508	3.6154753	-288439.97
BaO										
0	37643.985	-507.15553	5.3928473	-4.12E-04	-6.53E-07	9.43E-10	-3.44E-13	-12755.526	-3.7522138	-117948.39
1	1.32E+07	-38542.533	46.867416	-0.0218865	5.34E-06	-5.15E-10	1.43E-14	230690.24	-302.83328	-117948.39
2	-1.10E+09	356145.17	-12.362581	-0.0028129	3.31E-07	-1.25E-11	1.70E-16	-3157682.5	206.72975	-117948.39
BaO+										
0	356641.097	-3779.2467	16.735441	-0.0130661	2.69E-06	4.04E-09	-2.02E-12	79832.685	-72.851186	511704.69
1	-331767.923	1594.2535	3.2272478	5.72E-04	-1.15E-07	1.38E-11	-6.38E-16	50252.476	14.090924	511704.69
2	-3283193.02	2046.0498	4.0482251	9.87E-05	7.76E-11	2.54E-13	-1.33E-18	44568.585	8.5286209	511704.69
BaOH										
0	37762.3151	-889.13902	9.531718	-0.0054588	4.94E-06	-1.81E-09	2.05E-13	-24418.53	-24.894102	-224256.51
1	2637336.694	-8365.4104	15.99804	-0.0050984	1.59E-06	-2.18E-10	1.08E-14	23935.506	-74.907058	-224256.51
BaOH+										
0	27976.32165	-768.07694	9.0529784	-0.0043686	3.52E-06	-8.39E-10	-6.48E-14	26232.808	-22.645616	202019.31
1	876673.843	-2335.8196	7.9731661	1.04E-04	-6.32E-08	1.03E-11	-5.74E-16	37725.175	-19.30805	202019.31
Ba(OH)2										
0	57028.149	-1577.3848	16.599353	-0.010396	9.66E-06	-3.67E-09	4.63E-13	-68351.589	-58.519117	-606666.47
1	1762908.112	-4676.2054	13.951355	2.05E-04	-1.26E-07	2.05E-11	-1.14E-15	-45459.644	-49.294572	-606666.47
BaS										
0	13770.75147	-329.35006	5.8115458	-0.002849	3.58E-06	-2.33E-09	6.17E-13	4964.4325	-3.4979538	38871.315
1	6104262.07	-22276.175	35.975135	-0.0215779	7.32E-06	-1.09E-09	5.88E-14	140413.8	-214.17762	38871.315
Ba2										
0	-12941.77083	-727.63301	14.648666	-0.0396633	5.90E-05	-4.24E-08	1.19E-11	43867.122	-41.456737	355964.34
1	216011.4547	195.06769	2.2536998	1.51E-04	-4.74E-08	7.05E-12	-3.55E-16	41677.63	23.759065	355964.34
Be										
0	-4.11E-04	5.36E-06	2.5	7.57E-11	-1.10E-13	8.00E-17	-2.30E-20	38222.646	2.146173	324000
1	-692628.584	2466.773	-0.9776613	0.0024589	-9.05E-07	1.59E-10	-9.42E-15	23002.129	26.232348	324000
2	4.15E+08	-225414.75	44.114379	-0.0030229	1.18E-07	-2.27E-12	1.20E-17	1866686.3	-375.23374	324000
Be+										
0	0	0	2.5	0	0	0	0	147152.86	2.8392287	1229701.3
1	-94781.3598	276.83254	2.1913884	1.65E-04	-4.28E-08	4.54E-12	-6.27E-17	145385.1	5.0555038	1229701.3
2	-2.15E+08	143056.81	-34.382099	0.0045684	-2.78E-07	8.41E-12	-9.93E-17	-976696.34	321.57584	1229701.3
Be++										
0	0	0	2.5	0	0	0	0	359227.92	2.1459902	2993001.5

1	0	0	2.5	0	0	0	0	359227.92	2.1459902	2993001.5
2	0	0	2.5	0	0	0	0	359227.92	2.1459902	2993001.5
BeBO2										
0	0	0	2.006912	0.0180448	-1.69E-05	6.09E-09	-1.73E-13	-59234.197	15.805557	-482003.11
1	0	0	6.9108376	0.0032669	-1.37E-06	2.56E-10	-1.77E-14	-60505.715	-9.1616581	-482003.11
BeBr										
0	37462.8806	-472.23391	5.039409	5.80E-04	-1.94E-06	1.79E-09	-5.67E-13	17231.357	-2.5739129	132446.31
1	821723.814	-2850.5093	8.017266	-0.0021057	6.85E-07	-9.99E-11	5.19E-15	32293.729	-23.268108	132446.31
BeBr2										
0	-21186.98678	209.03826	3.7311713	0.011155	-1.54E-05	1.05E-08	-2.85E-12	-30904.563	9.4589177	-234062.5
1	-104133.1811	-154.34431	7.6144654	-4.56E-05	1.00E-08	-1.15E-12	5.30E-17	-29845.276	-11.49361	-234062.5
BeCL										
0	20161.38947	-141.3989	2.8982238	0.0060699	-9.16E-06	6.61E-09	-1.86E-12	6626.6914	7.9001709	56693.107
1	280884.5146	-1103.1001	5.6711898	-5.44E-04	1.46E-07	-1.23E-11	9.90E-17	12246.498	-8.3823815	56693.107
BeCL+										
0	0	0	2.8965984	0.0051267	-6.44E-06	3.56E-09	-6.59E-13	116714.66	7.8372705	979083.09
1	0	0	5.38275	-0.0018471	1.11E-06	-1.70E-10	6.10E-15	115997.17	-5.0622414	979083.09
BeCLF										
0	0	0	4.1024381	0.0085017	-8.91E-06	4.01E-09	-5.16E-13	-70468.736	4.0991628	-573191.97
1	0	0	6.4402791	0.0011464	-4.85E-07	9.13E-11	-6.34E-15	-71059.771	-7.7286997	-573191.97
BeCL2										
0	-22299.57657	152.87817	3.7149947	0.0106778	-1.40E-05	9.07E-09	-2.35E-12	-45904.282	6.6825443	-361539.14
1	-115408.746	-248.43001	7.6856721	-7.44E-05	1.65E-08	-1.90E-12	8.80E-17	-44687.473	-15.003385	-361539.14
BeF										
0	-46644.9723	788.71789	-1.4633632	0.0138179	-1.59E-05	9.35E-09	-2.23E-12	-25226.275	31.976343	-170624.8
1	-185794.1543	47.760828	4.269986	2.31E-04	-6.66E-08	1.15E-11	-6.34E-16	-22579.51	-0.2184787	-170624.8
BeF2										
0	7490.27024	-287.80531	5.4347128	0.0039032	-2.21E-06	-1.97E-10	4.04E-13	-95916.156	-5.6166169	-796588.24
1	-64820.1807	-768.45561	8.0628608	-2.23E-04	4.89E-08	-5.59E-12	2.58E-16	-93954.955	-21.256603	-796588.24
BeH										
0	-1615.149125	-59.352861	4.5072691	-0.0052642	1.15E-05	-9.25E-09	2.70E-12	40301.93	-3.4851171	342252.1
1	-2424081.636	6597.3985	-3.6263165	0.0045796	-1.16E-06	1.30E-10	-5.29E-15	-2489.8462	52.160187	342252.1
BeH+										
0	-32206.1102	252.02296	3.2077196	-0.0021913	6.90E-06	-5.77E-09	1.66E-12	139253.07	3.3070448	1178219
1	462234.159	-1760.1696	5.3799056	2.74E-05	-1.17E-07	3.56E-11	-2.57E-15	151585.97	-13.692226	1178219
2	2.27E+08	-120764.65	26.308248	-0.0014021	3.76E-08	6.34E-14	-1.26E-17	1121142.1	-204.92397	1178219
BeH2										
0	-130245.8357	1920.4063	-6.6723828	0.0219266	-1.43E-05	2.84E-09	4.62E-13	4852.8663	58.616284	125520
1	433779.392	-3572.0265	10.005776	-9.62E-04	2.07E-07	-2.32E-11	1.06E-15	34110.548	-45.075771	125520
BeI										
0	35300.5481	-519.09503	5.7145052	-0.0014091	7.66E-07	-2.60E-11	-8.23E-14	26379.037	-5.1409978	207454.31
1	-532820.662	1139.4979	3.6291717	1.70E-04	1.07E-07	-3.59E-11	2.72E-15	15854.743	9.3709513	207454.31
BeI2										
0	359.272618	-48.66059	5.2415712	0.0078303	-1.17E-05	8.39E-09	-2.36E-12	-9333.2209	2.8963183	-64759.451
1	-93923.7284	-89.592144	7.5655548	-2.58E-05	5.61E-09	-6.36E-13	2.92E-17	-9814.7686	-9.0320428	-64759.451
BeN										
0	-42477.8363	759.01889	-1.5614692	0.0149695	-1.84E-05	1.15E-08	-2.90E-12	46830.033	32.56974	427000
1	-59096.9616	-307.86494	4.7279592	-3.93E-05	2.01E-08	-2.30E-12	1.07E-16	51560.957	-3.031378	427000
BeO										
0	-48694.5832	721.34736	-0.3784157	0.0087922	-7.07E-06	2.25E-09	-2.80E-14	11014.666	25.740812	128940.3
1	-3.50E+07	105585.95	-116.50117	0.0647737	-1.65E-05	2.01E-09	-9.43E-14	-657001.8	864.0898	128940.3
2	-7.44E+07	43096.653	-0.1019586	2.62E-04	-2.46E-08	1.12E-12	-1.83E-17	-340237.94	44.870402	128940.3
BeOH										
0	-38530.2452	449.80593	1.5320965	0.0129991	-1.71E-05	1.17E-08	-3.16E-12	-15590.466	15.455429	-99717.721
1	855033.031	-2646.5378	8.2047846	1.11E-05	-4.27E-08	7.93E-12	-4.65E-16	3121.2163	-25.716413	-99717.721
BeOH+										
0	71061.1916	-806.89816	5.6031078	0.0049321	-7.72E-06	5.91E-09	-1.70E-12	94407.824	-10.880999	759983.92
1	813487.439	-2814.6537	8.381145	-6.94E-05	-2.37E-08	5.68E-12	-3.58E-16	107312.99	-29.010933	759983.92
2	-6279111.75	2090.0442	7.0255599	5.49E-05	-3.45E-09	1.12E-13	-1.46E-18	69148.37	-17.324432	759983.92
Be(OH)2										
0	7863.08983	-739.71423	10.433033	0.0045142	-6.95E-06	5.78E-09	-1.73E-12	-75856.77	-33.014666	-638864.42
1	1722889.403	-5242.4772	14.868778	3.93E-05	-8.92E-08	1.63E-11	-9.51E-16	-46428.238	-64.76804	-638864.42
BeS										
0	-7390.57908	282.81348	0.6552019	0.0107601	-1.40E-05	8.82E-09	-2.11E-12	27515.933	19.804972	247095.31
1	-1.66E+07	54314.661	-63.518593	0.0396409	-1.08E-05	1.39E-09	-6.94E-14	-312155.96	480.34553	247095.31
Be2										
0	-158087.381	2035.5678	-3.6915806	0.0102882	-9.60E-06	4.71E-09	-9.37E-13	65269.684	48.79325	637543.32
1	101003.4484	141.42075	2.2920702	1.54E-04	-5.80E-08	1.00E-11	-5.68E-16	75501.397	12.387586	637543.32
Be2CL4										
0	121615.2589	-2000.8248	17.233843	0.0058104	-1.36E-05	1.16E-08	-3.55E-12	-92064.755	-61.379609	-819604.97
1	-335492.008	-231.61993	16.170479	-6.73E-05	1.47E-08	-1.67E-12	7.69E-17	-103107.52	-50.470105	-819604.97
Be2F4										
0	-6327.70187	-69.025337	5.4709372	0.0309734	-4.09E-05	2.67E-08	-6.94E-12	-210597.93	-0.2073546	-1731699.8
1	-368183.495	-943.91915	16.700999	-2.80E-04	6.18E-08	-7.08E-12	3.28E-16	-208904.57	-60.926658	-1731699.8
Be2O										
0	-426.367357	-115.95563	4.0826778	0.0101589	-1.33E-05	8.49E-09	-2.17E-12	-5362.2581	1.2537379	-37033.803
1	-141264.6378	-349.86446	7.7609327	-1.04E-04	2.31E-08	-2.66E-12	1.23E-16	-5172.3855	-18.548876	-37033.803
Be2OF2										
0	0	0	4.8600026	0.019439	-1.88E-05	7.10E-09	-3.72E-13	-147039.59	3.2417334	-1204597.8
1	0	0	10.311343	0.0029258	-1.25E-06	2.37E-10	-1.66E-14	-148446.23	-24.487683	-1204597.8
Be2O2										
0	-30317.1953	1163.3532	-8.733156	0.05372	-7.28E-05	4.89E-08	-1.31E-11	-55469.369	69.532826	-411635.31

1	-396057.664	-907.49488	10.671604	-2.67E-04	5.88E-08	-6.72E-12	3.11E-16	-48611.143	-36.165469	-411635.31
Be3O3										
0	-27380.72346	874.38326	-6.5996061	0.0653302	-8.76E-05	5.82E-08	-1.54E-11	-128467.9	58.372031	-1023720.6
1	-589080.936	-1392.8236	17.034507	-4.13E-04	9.11E-08	-1.04E-11	4.83E-16	-121904.55	-70.006145	-1023720.6
Be4O4										
0	-68932.5564	1687.5651	-14.796166	0.100732	-1.29E-04	8.24E-08	-2.11E-11	-207287.72	100.25073	-1649294.6
1	-884133.846	-2726.3942	24.029418	-8.11E-04	1.79E-07	-2.06E-11	9.55E-16	-192371.06	-113.66208	-1649294.6
Br										
0	-3700.29413	61.452157	2.0921207	0.0013768	-2.45E-06	2.05E-09	-5.14E-13	12425.086	8.9961663	111870
1	-4789717.21	16920.519	-20.240853	0.0139562	-3.66E-06	4.49E-10	-2.12E-14	-92070.546	166.16959	111870
2	-1.12E+08	63459.62	-8.6178743	0.0011801	-6.22E-08	1.74E-12	-2.09E-17	-501464.02	108.61363	111870
Br+										
0	39811.8742	-475.15815	4.734579	-0.0051693	5.91E-06	-2.89E-09	5.05E-13	152905.2	-5.7692832	1257927
1	1741149.829	-5455.4657	8.4706634	-0.0026835	6.59E-07	-7.95E-11	3.74E-15	185178.16	-36.37909	1257927
2	-6.17E+07	36417.042	-5.7397447	0.0010675	-7.13E-08	2.16E-12	-1.77E-17	-139976.75	79.315777	1257927
Br-										
0	0	0	2.5	0	0	0	0	-27084.927	5.4195562	-219000.47
1	0	0	2.5	0	0	0	0	-27084.927	5.4195562	-219000.47
2	0	0	2.5	0	0	0	0	-27084.927	5.4195562	-219000.47
BrCL										
0	16532.91583	-357.87693	5.7006222	-0.0022013	2.42E-06	-1.37E-09	3.23E-13	2252.6193	-4.1556636	14789.113
1	-128486.3067	-1138.3796	7.9640408	-0.0034381	1.52E-06	-2.76E-10	1.69E-14	5938.2643	-19.250448	14789.113
BrF										
0	38361.4319	-518.4612	5.4583271	-5.66E-04	-4.12E-07	7.86E-10	-3.04E-13	-5595.5399	-4.9011295	-58851.445
1	3771388.47	-12674.934	20.805559	-0.0102636	3.31E-06	-4.90E-10	2.65E-14	70626.097	-113.02536	-58851.445
BrF3										
0	111645.5127	-1959.4243	15.262201	-0.0079994	6.98E-06	-3.24E-09	6.16E-13	-23453.416	-55.226336	-255600
1	-188653.224	-82.45233	10.061807	-2.48E-05	5.48E-09	-6.28E-13	2.91E-17	-33868.004	-22.989374	-255600
BrF5										
0	221136.6805	-4024.8092	27.349002	-0.0183225	1.72E-05	-8.75E-09	1.86E-12	-35374.477	-124.42965	-428800
1	-375764.764	-157.58965	16.118698	-4.78E-05	1.06E-08	-1.22E-12	5.66E-17	-56672.668	-55.408393	-428800
BrO										
0	14554.31116	122.51524	-0.3058729	0.0211731	-3.49E-05	2.62E-08	-7.51E-12	13891.499	25.278674	125800
1	-2392612.795	6932.7931	-2.5131839	0.0034465	-7.57E-07	6.51E-11	-1.72E-15	-30844.991	53.610484	125800
OBrO										
0	34702.1323	-340.13418	3.9322516	0.0121594	-1.90E-05	1.40E-08	-3.99E-12	18759.558	6.3612352	151954.53
1	-162450.466	-145.36894	7.1058221	-4.14E-05	8.98E-09	-1.01E-12	4.64E-17	16500.754	-9.1118179	151954.53
BrOO										
0	-44176.199	495.96372	3.239885	0.0059415	-3.40E-06	-3.44E-11	4.81E-13	8815.222	16.074469	108000
1	6172.48348	-658.50497	7.4839553	-1.92E-04	4.23E-08	-4.84E-12	2.24E-16	14603.535	-9.8503802	108000
BrO3										
0	106390.1881	-1501.9288	9.7036574	0.008133	-1.53E-05	1.20E-08	-3.51E-12	32331.36	-27.351254	220820.69
1	-282285.1113	-235.89735	10.175253	-6.98E-05	1.54E-08	-1.75E-12	8.10E-17	24011.401	-25.881972	220820.69
Br2										
0	7497.04754	-235.08846	5.4919343	-0.0022276	2.93E-06	-1.95E-09	5.31E-13	3521.4751	-1.9641516	30910
1	-4311698.57	11112.686	-5.5557756	0.0036305	-2.75E-07	-6.22E-11	7.38E-15	-70365.842	78.78478	30910
BrBrO										
0	16174.98037	-246.44068	5.9128585	0.0049804	-8.10E-06	6.07E-09	-1.75E-12	19740.121	2.009705	168000
1	-85371.0175	-64.870461	7.0471594	-1.84E-05	3.99E-09	-4.50E-13	2.06E-17	18215.667	-3.1621861	168000
BrOBr										
0	64050.6891	-1062.7226	9.9078663	-0.0044705	3.91E-06	-1.81E-09	3.37E-13	16429.215	-23.503194	107639.01
1	-96866.6025	-39.573953	7.0294344	-1.17E-05	2.58E-09	-2.94E-13	1.36E-17	10769.423	-5.6977794	107639.01
C										
0	649.503147	-0.9649011	2.5046755	-1.28E-05	1.98E-08	-1.61E-11	5.31E-15	85457.631	4.7479243	716680
1	-128913.6472	171.95286	2.6460444	-3.35E-04	1.74E-07	-2.90E-11	1.64E-15	84105.979	4.1300474	716680
2	4.43E+08	-288601.84	77.371083	-0.0097153	6.65E-07	-2.23E-11	2.90E-16	2355273.4	-640.51232	716680
C+										
0	2258.535929	-1.5745757	2.5036377	-5.20E-06	4.52E-09	-2.18E-12	4.50E-16	216895.19	4.3456995	1809444.5
1	12551.12551	-34.118747	2.5433832	-2.81E-05	9.75E-09	-1.74E-12	1.25E-16	217100.18	4.0639135	1809444.5
2	561813.532	-6047.0589	5.8845415	-7.21E-04	6.82E-08	-2.60E-12	3.63E-17	258137.05	-22.800198	1809444.5
C-										
0	4.67129153	-0.0019862	2.5000086	-1.98E-08	2.48E-11	-1.61E-14	4.24E-18	70012.186	4.8795701	588314.24
1	4.25317572	5.78E-04	2.4999994	2.84E-10	-7.33E-14	9.48E-18	-4.83E-22	70012.172	4.8796242	588314.24
2	12.23289007	-0.0051962	2.5000013	-1.74E-10	1.21E-14	-4.25E-19	5.99E-24	70012.216	4.8796084	588314.24
CBr										
0	2940.17881	-140.41128	4.7544668	-1.65E-04	4.35E-08	5.91E-11	-2.89E-14	58384.042	0.7135469	490430.44
1	-47426.5247	56.931186	4.4301183	9.15E-05	-6.42E-09	1.44E-12	-2.61E-17	57192.061	2.9070872	490430.44
CBr2										
0	72483.2841	-1128.2813	9.8224245	-0.0038731	2.91E-06	-1.06E-09	1.30E-13	44377.81	-23.611883	336623.32
1	-744140.996	421.53628	8.7968065	-0.0027266	1.34E-06	-2.30E-10	1.34E-14	33646.222	-15.995715	336623.32
CBr3										
0	85636.8067	-1275.7847	11.171998	0.0023415	-6.54E-06	5.74E-09	-1.78E-12	32432.26	-27.66525	235000
1	-192512.2669	-132.79137	10.098502	-3.92E-05	8.61E-09	-9.83E-13	4.54E-17	25418.23	-18.671684	235000
CBr4										
0	102304.1073	-1735.5322	16.512749	-0.0031463	2.90E-07	1.36E-09	-6.44E-13	15004.706	-55.362431	79500
1	-206123.2831	-104.45811	13.077319	-3.07E-05	6.72E-09	-7.66E-13	3.53E-17	5613.3512	-32.834926	79500
CCL										
0	14990.28985	15.36122	2.1691638	0.007639	-1.10E-05	7.66E-09	-2.11E-12	59447.529	12.922637	502100
1	-169577.6738	220.09982	4.2006462	2.33E-04	-5.37E-08	7.39E-12	-2.70E-16	57378.636	2.9822869	502100
CCLBr3										
0	102155.7592	-1746.2249	15.98184	-0.0013501	-2.33E-06	3.20E-09	-1.15E-12	13419.408	-52.849038	65000
1	-228242.5521	-127.85657	13.094961	-3.78E-05	8.33E-09	-9.54E-13	4.42E-17	3931.3664	-33.155885	65000

CCL2										
0	74618.6809	-1027.4396	8.0106836	0.0017039	-5.05E-06	4.49E-09	-1.40E-12	31338.96	-17.130662	230000
1	1952527.106	-7197.819	16.426716	-0.0060344	1.90E-06	-2.59E-10	1.28E-14	69881.284	-75.005128	230000
CCL2Br2										
0	101848.127	-1740.8375	15.213323	0.0011283	-5.88E-06	5.66E-09	-1.82E-12	6918.488	-50.153492	10000
1	-255402.7577	-159.61745	13.118422	-4.71E-05	1.03E-08	-1.18E-12	5.45E-17	-2589.8219	-34.615701	10000
CCL3										
0	34144.7202	-554.79703	6.8455447	0.0124201	-2.04E-05	1.55E-08	-4.57E-12	9385.2015	-7.1436193	71100
1	2405028.603	-8014.8552	18.812047	-0.0051213	1.47E-06	-2.02E-10	1.06E-14	55835.829	-85.350911	71100
CCL3Br										
0	104963.3736	-1793.7822	14.892274	0.0023977	-7.79E-06	7.02E-09	-2.20E-12	909.90935	-50.582162	-43000
1	-277091.4947	-184.4185	13.137145	-5.46E-05	1.20E-08	-1.37E-12	6.35E-17	-8893.3599	-36.698238	-43000
CCL4										
0	109338.5626	-1861.7318	14.496325	0.0039495	-1.01E-05	8.65E-09	-2.64E-12	-4948.0062	-51.802859	-95600
1	-304307.8255	-216.81705	13.161324	-6.43E-05	1.42E-08	-1.62E-12	7.48E-17	-15123.201	-39.968455	-95600
CF										
0	-48565.9087	837.06685	-1.5860538	0.013733	-1.55E-05	8.90E-09	-2.08E-12	24192.095	33.711047	242300
1	-73030.1173	-310.43255	4.6875597	-1.75E-05	1.18E-08	-1.88E-12	1.90E-16	29349.029	-2.3217792	242300
CF+										
0	-59752.6053	927.6935	-1.8666223	0.0138435	-1.51E-05	8.52E-09	-1.96E-12	131290.92	34.120341	1136742.5
1	-80523.8068	-339.06807	4.7084195	-3.97E-05	2.50E-08	-5.24E-12	5.31E-16	137072.98	-3.9208584	1136742.5
CFBr3										
0	51502.3257	-936.61898	10.443373	0.0120516	-1.88E-05	1.34E-08	-3.73E-12	-12431.793	-23.643742	-120000
1	-272901.9621	-332.85918	13.248281	-9.93E-05	2.19E-08	-2.52E-12	1.17E-16	-17301.587	-36.268577	-120000
CFCL										
0	17947.57102	-129.01806	2.7934599	0.0132356	-1.82E-05	1.21E-08	-3.21E-12	2623.8196	11.667224	25872.113
1	1945366.777	-7156.8148	15.839352	-0.0053525	1.60E-06	-2.09E-10	9.98E-15	45199.215	-72.49953	25872.113
CFCLBr2										
0	58984.2873	-1050.6575	10.393148	0.0127379	-2.00E-05	1.44E-08	-4.00E-12	-18378.266	-24.1729	-175000
1	-296169.5804	-352.90241	13.263239	-1.05E-04	2.33E-08	-2.67E-12	1.24E-16	-23877.411	-36.848156	-175000
CFCL2										
0	26115.33165	-335.37548	4.0947754	0.0196022	-2.76E-05	1.88E-08	-5.05E-12	-12512.898	6.8702975	-105000
1	-265308.9592	-446.99038	10.33338	-1.33E-04	2.95E-08	-3.38E-12	1.57E-16	-13931.5	-25.568404	-105000
CFCL2Br										
0	65288.8575	-1135.0868	10.094472	0.0140159	-2.19E-05	1.57E-08	-4.37E-12	-25045.599	-24.506478	-235000
1	-321661.068	-388.11048	13.289597	-1.16E-04	2.56E-08	-2.94E-12	1.36E-16	-30976.173	-38.711326	-235000
CFCL3										
0	72393.166	-1228.3384	9.9090489	0.0149511	-2.34E-05	1.67E-08	-4.65E-12	-30323.13	-26.447293	-283700
1	-344247.069	-421.74795	13.314963	-1.26E-04	2.79E-08	-3.20E-12	1.48E-16	-36715.775	-41.570162	-283700
CF2										
0	-42846.9549	942.24135	-3.8384738	0.0284788	-3.62E-05	2.31E-08	-5.91E-12	-27799.376	46.675983	-186600
1	-1985921.862	4474.8611	2.0536779	0.0025421	-6.47E-07	7.99E-11	-3.82E-15	-54348.511	22.889955	-186600
CF2+										
0	-1283.891178	384.09974	-0.6091411	0.0189463	-2.22E-05	1.30E-08	-3.10E-12	111393.95	29.660359	948480.59
1	401459.501	-2428.6293	9.4725743	-0.0012667	3.20E-07	-3.43E-11	1.33E-15	126393.76	-30.056196	948480.59
CF2Br2										
0	12608.55554	-281.49555	5.0976174	0.0250266	-3.44E-05	2.30E-08	-6.08E-12	-46428.008	3.0964863	-380000
1	-332810.724	-618.30535	13.461552	-1.85E-04	4.09E-08	-4.70E-12	2.18E-16	-47152.693	-41.052631	-380000
CF2CL										
0	8914.19493	-17.683781	1.6069957	0.0247363	-3.27E-05	2.13E-08	-5.51E-12	-34273.084	19.296909	-275000
1	-280276.7108	-685.92205	10.51133	-2.05E-04	4.53E-08	-5.20E-12	2.41E-16	-33082.508	-28.74823	-275000
CF2CLBr										
0	26969.19535	-467.91544	5.2449948	0.0253007	-3.51E-05	2.35E-08	-6.25E-12	-51983.674	0.8522605	-435000
1	-359357.495	-653.69871	13.488047	-1.95E-04	4.33E-08	-4.97E-12	2.30E-16	-53652.867	-42.247229	-435000
CF2CL2										
0	38445.0996	-613.26453	5.2562017	0.0257648	-3.59E-05	2.41E-08	-6.40E-12	-57846.12	-1.8934313	-490800
1	-382846.555	-696.03151	13.519916	-2.08E-04	4.61E-08	-5.30E-12	2.46E-16	-60200.728	-44.824336	-490800
CF3										
0	-28950.93138	708.2591	-3.498745	0.0360053	-4.52E-05	2.83E-08	-7.12E-12	-60557.995	45.004364	-467400
1	-300992.5372	-1045.7742	10.778307	-3.11E-04	6.88E-08	-7.90E-12	3.67E-16	-54263.67	-34.16192	-467400
CF3+										
0	21928.82878	17.150788	0.51872	0.0244283	-2.87E-05	1.68E-08	-3.95E-12	49908.409	21.689285	423632.58
1	-237352.2001	-1280.2394	10.944105	-3.75E-04	8.26E-08	-9.45E-12	4.37E-16	54405.875	-36.723667	423632.58
CF3Br										
0	-5436.76574	124.32449	0.9233861	0.03481	-4.55E-05	2.93E-08	-7.55E-12	-80233.788	22.328906	-648800
1	-383419.421	-971.89278	13.724775	-2.90E-04	6.42E-08	-7.38E-12	3.42E-16	-77653.184	-47.173659	-648800
CF3CL										
0	17294.54028	-165.18678	1.5441945	0.0339574	-4.47E-05	2.89E-08	-7.46E-12	-85324.173	16.68147	-704200
1	-409136.054	-1013.1562	13.755489	-3.02E-04	6.69E-08	-7.69E-12	3.57E-16	-84166.526	-49.093989	-704200
CF4										
0	9815.34964	116.36607	-1.2885276	0.0395962	-5.00E-05	3.13E-08	-7.84E-12	-113896.08	29.387596	-933500
1	-416418.379	-1414.8993	14.051386	-4.20E-04	9.28E-08	-1.06E-11	4.94E-16	-109514.19	-54.872022	-933500
CH										
0	22205.64134	-340.53718	5.5313864	-0.0057949	7.97E-06	-4.47E-09	9.60E-13	72403.905	-9.1076361	597338
1	2060733.772	-5396.1296	7.8561879	-7.97E-04	1.76E-07	-1.98E-11	5.03E-16	106219.25	-31.54718	597338
2	-8.07E+08	457539.32	-98.438513	0.0123523	-8.49E-07	3.04E-11	-4.40E-16	-3595809.6	895.33644	597338
CH+										
0	30195.67	-461.80814	6.2255643	-0.0077756	1.09E-05	-6.68E-09	1.57E-12	197244.49	-14.315014	1630532
1	-7102008.54	18283.327	-13.126755	0.0061916	-2.91E-07	-1.13E-10	1.11E-14	75409.732	124.39691	1630532
2	-3.16E+08	143668.27	-11.084312	1.56E-04	4.93E-08	-2.90E-12	4.98E-17	-1013663.5	148.93356	1630532
CHBr3										
0	43461.3043	-499.89993	5.6198706	0.0207944	-2.92E-05	2.07E-08	-5.78E-12	2622.7146	1.2498575	16700

1	627412.218	-3378.6792	14.878491	-5.93E-04	1.08E-07	-1.06E-11	4.32E-16	18767.331	-53.118848	16700
CHCL										
0	-13516.85347	504.52044	-1.2381747	0.0211863	-3.14E-05	2.45E-08	-7.26E-12	32472.86	31.79809	297100
1	9452674.48	-27738.258	33.053177	-0.0104908	2.19E-06	-2.31E-10	9.76E-15	212103.95	-207.29128	297100
CHCLBr2										
0	38156.6479	-408.46063	4.6394982	0.0232592	-3.22E-05	2.25E-08	-6.26E-12	1484.0131	6.1738325	10000
1	604353.962	-3438.4183	14.941805	-6.23E-04	1.15E-07	-1.15E-11	4.73E-16	18225.761	-54.073892	10000
CHCL2										
0	56385.5597	-656.24551	6.0688179	0.0097441	-1.28E-05	8.55E-09	-2.23E-12	13304.478	-4.533556	95800
1	884940.301	-3526.972	11.863724	-5.00E-04	6.13E-08	-1.89E-12	-1.23E-16	30711.379	-40.889096	95800
CHCL2Br										
0	32939.3613	-327.51932	3.7731868	0.0253648	-3.47E-05	2.40E-08	-6.62E-12	-5425.6186	9.4336864	-45000
1	592475.941	-3509.4282	14.993431	-6.43E-04	1.20E-07	-1.20E-11	4.97E-16	11972.223	-56.026433	-45000
CHCL3										
0	33953.9304	-304.75071	2.9237096	0.0283054	-3.71E-05	2.55E-08	-6.99E-12	-12350.593	11.155334	-102700
1	613421.884	-3714.5551	15.107183	2.37E-04	1.30E-07	-1.27E-11	5.25E-16	6199.9118	-59.921544	-102700
CHF										
0	-45387.0807	873.46853	-1.9737247	0.017174	-1.93E-05	1.28E-08	-3.40E-12	7928.6369	36.40756	108800
1	7670328.62	-22860.739	27.688214	-0.0077522	1.51E-06	-1.59E-10	6.92E-15	158010.81	-170.38588	108800
CHFBr2										
0	-18204.96548	436.26689	-0.3736145	0.0338869	-4.37E-05	2.89E-08	-7.68E-12	-24656.318	33.206062	-175000
1	593568.248	-3742.6503	15.171848	-7.16E-04	1.36E-07	-1.39E-11	5.85E-16	-2347.7297	-57.657879	-175000
CHFCL										
0	-71130.3304	1377.8758	-6.4846319	0.0389098	-4.80E-05	3.07E-08	-7.98E-12	-17517.953	63.73903	-83144.704
1	662150.121	-3808.8231	12.238607	-7.47E-04	1.43E-07	-1.48E-11	6.27E-16	10188.689	-46.582241	-83144.704
CHFCLBr										
0	-19595.16997	490.20992	-1.2596054	0.0361776	-4.65E-05	3.07E-08	-8.12E-12	-31399.189	37.10561	-230000
1	579894.586	-3823.0113	15.227742	-7.37E-04	1.41E-07	-1.44E-11	6.08E-16	-8554.3509	-59.034268	-230000
CHFCL2										
0	-17887.03489	497.48366	-1.8714791	0.0378347	-4.86E-05	3.19E-08	-8.45E-12	-37913.178	38.105902	-284900
1	565697.196	-3891.9927	15.278812	-7.58E-04	1.45E-07	-1.49E-11	6.32E-16	-14814.785	-61.707252	-284900
CHF2										
0	-146969.0135	2553.3973	-13.026276	0.0543813	-6.71E-05	4.29E-08	-1.11E-11	-41793.722	99.399285	-238900
1	552681.191	-3696.0104	12.086107	-6.50E-04	1.12E-07	-9.81E-12	3.35E-16	-9437.0602	-47.044189	-238900
CHF2Br										
0	-77147.1599	1422.5753	-6.6845785	0.0473844	-5.83E-05	3.70E-08	-9.50E-12	-58785.157	66.087404	-422000
1	576732.196	-4177.6109	15.501397	-8.49E-04	1.66E-07	-1.73E-11	7.43E-16	-29662.153	-63.493014	-422000
CHF2CL										
0	-71535.7492	1355.1236	-7.1238804	0.0485476	-5.96E-05	3.76E-08	-9.61E-12	-65605.436	66.374897	-482800
1	562266.841	-4293.1004	15.57621	-8.76E-04	1.71E-07	-1.79E-11	7.72E-16	-36374.006	-66.071308	-482800
CHF3										
0	-109513.4981	2042.275	-11.662118	0.057858	-6.86E-05	4.21E-08	-1.05E-11	-93954.709	89.359151	-693300
1	568593.953	-4728.5697	15.867519	-7.38E-04	1.97E-07	-2.06E-11	8.97E-16	-59230.637	-71.614416	-693300
CH2										
0	35259.1418	-336.76544	4.5089369	0.0025211	-5.31E-06	6.65E-09	-2.61E-12	47377.255	-3.8074043	388800
1	2510415.94	-7953.9324	12.388296	-0.0017759	3.22E-07	-3.07E-11	1.20E-15	96010.286	-61.559844	388800
CH2Br2										
0	4793.75215	361.43368	-1.8198376	0.0347711	-4.50E-05	3.07E-08	-8.43E-12	-4485.3374	38.272618	-14800
1	1528243.72	-6673.3021	16.702011	-0.0011663	2.12E-07	-2.08E-11	8.43E-16	36002.733	-74.479777	-14800
CH2CL										
0	-31887.7225	633.34174	-1.164198	0.0216062	-2.55E-05	1.69E-08	-4.66E-12	10201.302	32.309092	119200
1	1662402.02	-6441.0347	13.597453	-0.0011405	2.09E-07	-2.05E-11	8.38E-16	52128.465	-61.485247	119200
CH2CLBr										
0	-13085.60298	645.67283	-3.5778293	0.0383382	-4.86E-05	3.26E-08	-8.85E-12	-9402.689	47.490728	-45000
1	1525025.678	-6823.3601	16.827721	-0.0012198	2.25E-07	-2.22E-11	9.11E-16	33202.565	-76.375931	-45000
CH2CL2										
0	-25097.41052	868.75225	-5.0945882	0.0415003	-5.20E-05	3.45E-08	-9.27E-12	-16389.719	53.968437	-95000
1	1529283.055	-6976.9704	16.941568	-0.0012651	2.34E-07	-2.33E-11	9.63E-16	28063.279	-79.494688	-95000
CH2F										
0	-85697.1323	1392.2268	-4.3820531	0.0264592	-2.85E-05	1.73E-08	-4.44E-12	-11694.446	50.494968	-31800
1	-3.59E+08	921130.49	-887.42977	0.4271265	-1.06E-04	1.32E-08	-6.50E-13	-6015409.5	6529.0986	-31800
CH2FBr										
0	-92561.3971	1811.9901	-9.69837	0.0503585	-6.07E-05	3.88E-08	-1.01E-11	-35375.117	81.404086	-215000
1	1539996.347	-7231.62	17.14575	-0.0013502	2.54E-07	-2.56E-11	1.07E-15	15096.472	-80.621148	-215000
CH2FCl										
0	-107485.3941	2089.1589	-11.619113	0.0546301	-6.55E-05	4.16E-08	-1.08E-11	-42681.993	90.684547	-265700
1	1533648.782	-7369.6607	17.251454	-0.0013931	2.63E-07	-2.67E-11	1.12E-15	9754.4636	-83.08255	-265700
CH2F2										
0	-181992.2125	3174.4334	-17.142592	0.0641136	-7.31E-05	4.43E-08	-1.10E-11	-70270.617	120.73332	-452300
1	1546546.355	-7876.7038	17.687505	-0.0015812	3.07E-07	-3.18E-11	1.36E-15	-9801.2853	-89.072781	-452300
CH3										
0	-28772.8611	509.50561	0.1990731	0.0136397	-1.43E-05	1.01E-08	-3.03E-12	14110.987	20.233886	146900
1	2760904.27	-9336.5528	14.876986	-0.0014392	2.44E-07	-2.22E-11	8.39E-16	74847.648	-79.194893	146900
CH3Br										
0	-71155.9799	1524.7072	-8.230449	0.0423997	-4.95E-05	3.19E-08	-8.53E-12	-12512.732	70.481354	-37700
1	2524823.219	-10118.622	18.658879	-0.0017976	3.30E-07	-3.25E-11	1.33E-15	55409.679	-97.785555	-37700
CH3CL										
0	-98419.8777	1983.7023	-10.845126	0.0477798	-5.52E-05	3.51E-08	-9.24E-12	-19946.903	83.996587	-81870
1	2522470.775	-10301.182	18.827295	-0.0018723	3.47E-07	-3.46E-11	1.43E-15	51114.342	-100.65741	-81870
CH3F										
0	-202982.5364	3447.3358	-17.689967	0.0594528	-6.47E-05	3.86E-08	-9.63E-12	-45779.285	122.83834	-237700
1	2561892.955	-10860.512	19.294467	-0.002071	3.93E-07	-3.99E-11	1.68E-15	35634.972	-106.11583	-237700

CH2OH										
0	-82331.7198	1300.5364	-4.1663784	0.0303393	-3.41E-05	2.18E-08	-5.79E-12	-8602.0101	49.261769	-8900
1	2528592.31	-9235.952	17.129085	-0.0013108	2.14E-07	-1.87E-11	6.85E-16	54183.956	-86.74895	-8900
CH3O										
0	-28296.2698	676.19633	-2.2791657	0.0242334	-2.21E-05	1.23E-08	-3.10E-12	-2609.2915	36.337858	13000
1	2224626.76	-9720.5655	18.82482	-0.0019615	3.79E-07	-3.96E-11	1.79E-15	58429.319	-100.41681	13000
CH4										
0	-176654.573	2785.4778	-12.019355	0.0391463	-3.61E-05	2.02E-08	-4.96E-12	-23310.116	89.010754	-74600
1	3746265.7	-13888.513	20.540298	-0.0019442	4.32E-07	-4.06E-11	1.64E-15	75659.887	-122.29777	-74600
CH3OH										
0	-241663.747	4032.1381	-20.464095	0.0690368	-7.60E-05	4.60E-08	-1.16E-11	-44332.57	140.01389	-200940
1	3411560.75	-13454.975	22.614046	-0.002141	3.73E-07	-3.50E-11	1.37E-15	56360.639	-127.78123	-200940
CI										
0	103586.225	-1705.7814	12.838201	-0.0181474	2.12E-05	-1.27E-08	3.13E-12	75460.878	-44.684499	570200.66
1	-27181.7224	203.00287	4.348516	1.27E-04	-1.05E-08	1.57E-12	-7.18E-17	65995.858	4.6515623	570200.66
CN										
0	3949.10175	-139.15739	4.930776	-0.0063046	1.26E-05	-9.88E-09	2.84E-12	52284.547	-2.7631146	438683.45
1	-2227976.079	5040.6645	-0.2121794	0.0013549	1.33E-07	-6.94E-11	5.49E-15	17845.423	32.825155	438683.45
2	-1.79E+08	105433.14	-17.295989	0.0021949	-8.51E-08	9.32E-13	6.36E-18	-796247.65	191.31124	438683.45
CN+										
0	-830280.101	8775.572	-29.774032	0.0497683	-1.30E-05	-2.06E-08	1.13E-11	170579.09	203.98914	1800490.9
1	-7153374.51	18572.275	-10.845205	0.0061066	-1.19E-06	1.18E-10	-4.80E-15	92620.412	113.53262	1800490.9
2	-1.81E+08	112880.45	-22.873084	0.0034846	-2.21E-07	6.58E-12	-7.56E-17	-678420.86	236.26335	1800490.9
CN-										
0	-45944.1773	426.66177	2.3476244	-1.81E-04	4.57E-06	-4.47E-09	1.37E-12	4566.9713	11.327224	65485.578
1	347882.458	-1621.468	5.6024587	-3.94E-04	8.73E-08	-9.68E-12	4.38E-16	16612.271	-11.699386	65485.578
CNN										
0	-1347.06957	-138.4816	4.5917604	0.004297	-4.27E-06	2.94E-09	-8.91E-13	75445.829	0.1609001	633474.7
1	608532.725	-2582.4351	8.6949262	-1.83E-04	-1.36E-08	8.58E-12	-5.81E-16	90212.15	-27.213433	633474.7
CO										
0	14890.27557	-292.22509	5.7244584	-0.0081761	1.46E-05	-1.09E-08	3.03E-12	-13030.697	-7.8591793	-110530
1	461915.856	-1944.6857	5.9166471	-5.66E-04	1.40E-07	-1.79E-11	9.62E-16	-2465.7384	-13.874026	-110530
2	8.87E+08	-750028.54	249.54445	-0.039563	3.30E-06	-1.32E-10	2.00E-15	5701351.2	-2060.6796	-110530
CO+										
0	-21787.3999	128.88182	3.7690229	-0.0034317	8.19E-06	-6.46E-09	1.80E-12	148234.83	3.9904057	1247790.9
1	231681.66	-1057.6326	4.5542023	4.50E-04	-2.49E-07	5.27E-11	-3.29E-15	155505.2	-3.873443	1247790.9
2	-3.04E+08	239308.39	-70.34902	0.0113954	-8.32E-07	2.86E-11	-3.80E-16	-1688590.8	629.18933	1247790.9
COCL										
0	25131.89017	-596.92237	8.3277005	-0.0070562	1.31E-05	-1.04E-08	3.03E-12	-705.26241	-15.807333	-16000
1	344320.857	-1793.0027	8.3926069	-5.37E-04	9.11E-08	-3.11E-12	-2.04E-16	6913.5629	-19.988129	-16000
COCL2										
0	93190.104	-1577.9291	12.08332	-0.0048085	7.69E-06	-5.86E-09	1.69E-12	-20542.728	-38.346454	-219500
1	-25461.27725	-1305.9434	10.929198	-3.60E-04	7.79E-08	-8.79E-12	4.03E-16	-22198.561	-32.332863	-219500
COF										
0	12157.78086	-65.935266	3.0215511	0.007488	-6.17E-06	2.39E-09	-3.36E-13	-22345.659	10.615862	-179413.27
1	208436.5824	-1775.4629	8.3200921	-4.82E-04	7.39E-08	-1.04E-12	-2.88E-16	-13203.496	-22.033923	-179413.27
COFCL										
0	72621.6096	-1019.7375	7.2909161	0.0074207	-7.90E-06	4.21E-09	-9.31E-13	-48043.869	-13.169262	-429492.86
1	-53208.5991	-1580.8983	11.126844	-4.37E-04	9.46E-08	-1.07E-11	4.90E-16	-45997.388	-35.25794	-429492.86
COF2										
0	52634.1656	-461.864	2.7741369	0.0183192	-2.13E-05	1.27E-08	-3.10E-12	-75642.534	9.4670525	-640000
1	-40728.5282	-1974.0368	11.403665	-5.44E-04	1.18E-07	-1.33E-11	6.08E-16	-69077.781	-40.097164	-640000
COHCL										
0	6331.74919	81.220237	1.3745593	0.0165099	-1.69E-05	9.68E-09	-2.37E-12	-21203.646	19.384281	-164211.88
1	831883.551	-4416.8437	12.706587	-9.36E-04	1.86E-07	-1.96E-11	8.51E-16	4330.3166	-51.450554	-164211.88
COHF										
0	-45859.1407	1048.2136	-4.7766262	0.0308073	-3.42E-05	2.03E-08	-5.05E-12	-50859.891	52.322763	-374590.36
1	857899.885	-4791.9993	12.939794	-0.0010183	2.02E-07	-2.14E-11	9.30E-16	-18789.072	-55.274804	-374590.36
COS										
0	85479.4437	-1319.4736	9.7353004	-0.0068709	1.08E-05	-7.71E-09	2.08E-12	-11916.534	-29.920114	-141700
1	195869.6362	-1756.0611	8.7103218	-4.14E-04	1.02E-07	-1.16E-11	5.69E-16	-8927.7874	-26.362475	-141700
CO2										
0	49437.8364	-626.42921	5.3018134	0.0025036	-2.12E-07	-7.69E-10	2.85E-13	-45281.899	-7.0487901	-393510
1	117696.9434	-1788.8015	8.2915435	-9.22E-05	4.87E-09	-1.89E-12	6.33E-16	-39083.45	-26.52684	-393510
2	-1.54E+09	1016836.1	-256.13771	0.0336936	-2.18E-06	6.99E-11	-8.84E-16	-8043128.5	2254.1532	-393510
CO2+										
0	-73830.6812	1086.2181	-2.7711503	0.0231847	-2.57E-05	1.45E-08	-3.33E-12	107178.09	40.549049	944684.91
1	-169511.496	-806.62623	8.0028021	-1.58E-04	2.57E-08	-2.40E-12	1.68E-16	115438.45	-21.335503	944684.91
2	-8.36E+07	53323.286	-5.6191979	0.0014911	-7.55E-08	1.79E-12	-1.63E-17	-311113.14	96.717225	944684.91
COOH										
0	-11286.7245	377.55956	-0.5994864	0.0218196	-2.43E-05	1.45E-08	-3.60E-12	-28410.625	29.346893	-213000
1	929306.699	-4483.0005	12.421968	-7.46E-04	1.33E-07	-1.28E-11	5.14E-16	-852.0207	-50.680461	-213000
CP										
0	-45154.5447	774.96054	-1.4504133	0.0139716	-1.62E-05	9.52E-09	-2.21E-12	57930.694	33.095365	520158.8
1	-5646862.02	17362.807	-16.330599	0.0114335	-2.82E-06	3.29E-10	-1.48E-14	-48723.166	148.01135	520158.8
CS										
0	-49249.1322	816.70658	-1.5430519	0.0138034	-1.57E-05	9.17E-09	-2.17E-12	28798.73	33.085735	279771.88
1	-971961.2	2339.2091	1.7093851	0.0015772	-4.15E-07	4.50E-11	-5.95E-16	16957.102	18.740547	279771.88
CS2										
0	16132.8708	-464.9089	6.2977198	0.0018895	3.02E-07	-1.74E-09	7.79E-13	14777.423	-9.302132	116700
1	-1390420.939	3354.97	3.0192638	0.0028764	-9.08E-07	1.37E-10	-7.00E-15	-10138.955	15.651065	116700
C2										

0	555956.757	-9980.0062	66.815399	-0.1743412	2.45E-04	-1.70E-07	4.68E-11	144586.39	-344.81889	830457
1	-968890.957	3560.9902	-0.5063512	0.0029451	-7.14E-07	8.67E-11	-4.08E-15	76818.6	33.398961	830457
2	6316167.42	13653.441	-3.9967232	0.0019375	-1.58E-07	5.52E-12	-7.25E-17	9392.9053	66.141268	830457
C2+										
0	-99133.3666	1347.1581	-3.4767281	0.0167641	-1.87E-05	1.09E-08	-2.43E-12	233545.54	44.065937	2004775.4
1	3836171.46	-6241.7871	2.7790004	0.0060659	-2.45E-06	3.88E-10	-2.19E-14	285742.91	0.7311801	2004775.4
2	4.99E+07	-20176.83	6.3430441	6.37E-04	-1.04E-07	4.94E-12	-7.99E-17	412115.62	-21.137308	2004775.4
C2-										
0	-118191.339	1438.1712	-3.1960875	0.0146553	-1.55E-05	9.06E-09	-2.14E-12	49653.294	42.255474	480767
1	4478264.21	-11541.809	13.101797	-0.001863	4.01E-08	3.71E-11	-3.34E-15	132537.9	-69.762626	480767
C2CL										
0	47259.9592	-898.03861	9.0169734	-0.0063341	1.09E-05	-8.09E-09	2.25E-12	67022.234	-23.549486	534083.07
1	213701.7514	-1630.43	8.6234072	-4.25E-04	9.04E-08	-1.01E-11	4.57E-16	71710.347	-24.129555	534083.07
C2CL2										
0	38701.5433	-933.54081	11.192956	-0.003744	6.77E-06	-4.91E-09	1.30E-12	26281.606	-33.102693	200000
1	296148.2255	-2044.1679	11.875186	-5.11E-04	1.07E-07	-1.18E-11	5.33E-16	33167.989	-40.007457	200000
C2CL3										
0	46744.5017	-885.01732	9.0317769	0.0124227	-1.55E-05	9.52E-09	-2.34E-12	24958.232	-17.787998	190271.59
1	-220357.0165	-1073.0855	13.783883	-3.09E-04	6.78E-08	-7.73E-12	3.57E-16	24311.19	-43.423102	190271.59
C2CL4										
0	37462.6554	-848.17096	10.091474	0.018455	-2.39E-05	1.51E-08	-3.84E-12	-10.725617	-23.680382	-11000
1	-300231.185	-1132.1378	16.830441	-3.29E-04	7.22E-08	-8.24E-12	3.81E-16	-706.95521	-59.799569	-11000
C2CL6										
0	159352.807	-2606.8035	20.280697	0.0176921	-3.13E-05	2.39E-08	-6.89E-12	-8231.675	-79.533969	-141500
1	-557576.648	-497.98827	22.370664	-1.48E-04	3.26E-08	-3.73E-12	1.72E-16	-22544.119	-83.819204	-141500
C2F										
0	12496.3839	-348.36518	5.7549615	8.53E-04	2.35E-06	-2.80E-09	9.08E-13	42815.145	-6.4365361	353847.48
1	289878.0324	-2016.6544	8.8750663	-5.17E-04	1.09E-07	-1.21E-11	5.48E-16	52412.932	-27.731055	353847.48
C2FCL										
0	26982.13892	-741.52003	9.6300649	-3.88E-04	3.01E-06	-2.71E-09	7.74E-13	5500.9994	-25.160308	33766.399
1	347134.329	-2348.4395	12.068752	-5.80E-04	1.21E-07	-1.33E-11	5.99E-16	15020.46	-42.524421	33766.399
C2FCL3										
0	12372.04342	-470.38746	7.5815895	0.0230573	-2.79E-05	1.68E-08	-4.08E-12	-20313.384	-9.2744553	-166000
1	-283041.9579	-1473.6226	17.078563	-4.26E-04	9.35E-08	-1.07E-11	4.93E-16	-17385.838	-61.968909	-166000
C2F2										
0	17765.6119	-611.36483	8.6638192	9.15E-04	2.36E-06	-2.75E-09	8.72E-13	-16495.936	-21.65269	-144665.69
1	419277.332	-2715.0299	12.303661	-6.65E-04	1.38E-07	-1.52E-11	6.81E-16	-4181.3263	-46.701206	-144665.69
C2F2CL2										
0	-115043.2931	2032.1126	-11.197493	0.0834245	-1.16E-04	7.83E-08	-2.07E-11	-52082.564	88.883161	-337837
1	-870205.868	726.31909	15.307069	3.04E-04	-7.04E-08	8.28E-12	-3.90E-16	-52087.913	-49.984288	-337837
C2F3										
0	-26145.89241	210.14846	2.3287931	0.0236889	-2.42E-05	1.22E-08	-2.49E-12	-30285.532	16.995154	-228181.09
1	-124292.5975	-2137.2016	14.55041	-6.09E-04	1.33E-07	-1.51E-11	6.98E-16	-19772.043	-54.209672	-228181.09
C2F3CL										
0	-8122.99251	-157.39314	5.0417857	0.0262169	-2.84E-05	1.54E-08	-3.36E-12	-63540.539	2.792445	-515200
1	-216188.8941	-2195.3506	17.596326	-6.28E-04	1.37E-07	-1.57E-11	7.22E-16	-55149.516	-69.221287	-515200
C2F4										
0	-9991.35933	-129.11484	4.5042845	0.0259201	-2.63E-05	1.32E-08	-2.62E-12	-80904.446	3.2739474	-659500
1	-162934.8913	-2604.0722	17.885081	-7.40E-04	1.61E-07	-1.84E-11	8.46E-16	-70062.648	-74.543066	-659500
C2F6										
0	-37962.3266	799.95222	-4.6722629	0.0750165	-9.81E-05	6.32E-08	-1.62E-11	-167521.78	50.541474	-1344000
1	-1011461.523	-942.47201	22.025826	-1.32E-04	1.87E-08	-3.47E-12	2.49E-16	-165741.79	-93.023675	-1344000
C2H										
0	7653.69105	-418.74013	7.2542719	-0.005037	8.24E-06	-4.62E-09	9.51E-13	68506.897	-15.860356	566205.47
1	3995864.09	-11969.093	17.13833	-0.003337	6.00E-07	-5.50E-11	2.02E-15	143142.32	-92.859259	566205.47
C2HCL										
0	132974.3656	-2174.484	14.979491	-0.0129026	1.60E-05	-9.15E-09	2.02E-12	34418.867	-59.580624	212856.78
1	1152211.658	-4461.3911	12.813895	-6.80E-04	1.15E-07	-1.05E-11	3.95E-16	50711.869	-53.208187	212856.78
C2HCL3										
0	39586.6505	-517.79544	5.1545887	0.0281704	-3.62E-05	2.39E-08	-6.36E-12	-1727.1648	1.2118168	-19100
1	604945.033	-4237.0852	18.462879	-8.14E-04	1.55E-07	-1.59E-11	6.70E-16	18290.978	-76.984684	-19100
C2HF										
0	91607.1219	-1537.1804	11.336288	-0.0046237	5.88E-06	-2.69E-09	3.52E-13	10858.716	-40.23795	41692.304
1	1234330.392	-4819.5382	13.023335	-7.50E-04	1.29E-07	-1.18E-11	4.54E-16	32367.832	-56.407628	41692.304
C2HFCL2										
0	31171.08411	-136.90954	1.1761769	0.0408084	-5.42E-05	3.61E-08	-9.63E-12	-21151.626	21.465561	-168648
1	407176.189	-3808.3508	18.2116	-7.28E-04	1.38E-07	-1.41E-11	5.92E-16	-2675.9113	-75.674699	-168648
C2HF2CL										
0	170439.3681	-1667.1748	4.7884482	0.0444492	-7.32E-05	5.63E-08	-1.65E-11	-32918.396	-5.7867114	-333654
1	583029.12	-3810.2878	17.989992	-5.89E-04	1.00E-07	-9.15E-12	3.46E-16	-22058.937	-75.909221	-333654
C2HF3										
0	-14114.68689	368.83297	-1.1451835	0.0395641	-4.60E-05	2.79E-08	-6.90E-12	-62264.442	32.898757	-491000
1	691707.965	-5260.2218	19.152695	-0.0010725	2.10E-07	-2.20E-11	9.47E-16	-32476.929	-87.504052	-491000
CHCO,ketyl										
0	55952.7045	-913.44096	8.5828355	-0.0042454	7.21E-06	-3.43E-09	4.10E-13	22338.531	-21.007922	161084
1	2154213.19	-7508.8922	14.079026	-0.0012569	2.24E-07	-2.14E-11	8.49E-16	64564.783	-65.049519	161084
C2H2,vinylidene										
0	-14659.4987	278.9342	1.2763048	0.0139499	-1.48E-05	9.48E-09	-2.57E-12	47361.142	16.581806	414788.17
1	1940844.95	-6892.7445	13.395862	-9.37E-04	1.47E-07	-1.22E-11	4.12E-16	91071.266	-63.375324	414788.17
C2H2,acetylene										
0	159813.325	-2216.6751	12.657256	-0.0079802	8.06E-06	-2.43E-09	-7.51E-14	37126.338	-52.444406	228200
1	1713792.12	-5928.971	12.361156	1.31E-04	-1.36E-07	2.71E-11	-1.30E-15	62664.897	-58.188729	228200

C2H2CL2										
0	-12037.74009	462.90976	-1.3182186	0.0393046	-4.85E-05	3.18E-08	-8.48E-12	-3251.8391	34.892355	3410
1	1561078.805	-7357.982	20.118575	-0.0013109	2.41E-07	-2.38E-11	9.78E-16	41221.269	-95.501699	3410
C2H2FCL										
0	226014.1265	-2557.4125	9.2361681	0.0287942	-5.16E-05	4.25E-08	-1.31E-11	-8180.7087	-32.347467	-165082
1	1527659.307	-6689.6307	19.505458	-0.0010409	1.78E-07	-1.63E-11	6.21E-16	17052.133	-91.940216	-165082
C2H2F2										
0	57028.2573	-676.27041	4.1173259	0.0182264	-6.86E-06	-3.30E-09	2.18E-12	-38386.583	1.4879931	-336400
1	-822802.103	-2915.4933	18.301405	-0.0010395	2.55E-07	-3.16E-11	1.55E-15	-31101.742	-84.00666	-336400
CH2CO,ketene										
0	35096.1366	-401.03027	3.6959822	0.0158857	-1.73E-05	1.16E-08	-3.31E-12	-5010.6695	2.8241732	-47700
1	2015808.05	-8201.8983	17.590961	-0.0014606	2.69E-07	-2.65E-11	1.09E-15	42016.365	-88.369829	-47700
C2H3,vinyl										
0	-14479.5953	814.30434	-5.3133317	0.0376124	-4.60E-05	3.10E-08	-8.58E-12	31623.467	51.625887	299740.15
1	2561698.63	-10057.947	18.518745	-0.0017192	3.09E-07	-2.99E-11	1.20E-15	95758.745	-98.184851	299740.15
C2H3CL										
0	-16890.84887	854.53572	-6.5150972	0.0494472	-6.12E-05	4.07E-08	-1.10E-11	-1949.1726	59.285062	23000
1	2456166.38	-10474.494	21.78733	-0.0018169	3.30E-07	-3.21E-11	1.30E-15	63582.37	-114.98885	23000
C2H3F										
0	-45791.9009	1411.5491	-10.215047	0.0577583	-7.08E-05	4.64E-08	-1.24E-11	-24027.924	78.608479	-140100
1	2478832.992	-10759.338	21.947997	-0.0018691	3.40E-07	-3.32E-11	1.35E-15	45634.637	-118.04125	-140100
CH3CN										
0	-98761.9542	1719.3905	-7.7433143	0.0424184	-4.42E-05	2.66E-08	-6.86E-12	-1614.1194	67.702606	64430
1	2931022.01	-12365.4	23.266733	-0.0024214	4.65E-07	-4.77E-11	2.03E-15	80520.643	-129.40262	64430
CH3CO,acetyl										
0	-71940.0608	1464.481	-6.6323645	0.0410849	-4.23E-05	2.49E-08	-6.29E-12	-9309.447	64.229446	-10000
1	2485510.168	-11207.478	22.775609	-0.0023144	4.54E-07	-4.74E-11	2.05E-15	63803.047	-121.53767	-10000
C2H4										
0	-116361.327	2554.8605	-16.097503	0.0662579	-7.89E-05	5.13E-08	-1.37E-11	-6176.2361	109.33403	52500
1	3408725.12	-13748.364	23.658848	-0.0024237	4.43E-07	-4.35E-11	1.78E-15	88203.563	-137.1269	52500
C2H4O,ethylen-o										
0	-172824.024	3816.6888	-26.298575	0.1014105	-1.24E-04	8.03E-08	-2.12E-11	-24375.241	165.48879	-52634.72
1	3151847.33	-14236.576	27.080936	-0.0026063	4.85E-07	-4.85E-11	2.01E-15	76626.332	-156.3962	-52634.72
CH3CHO,ethanal										
0	-137392.192	2559.9613	-13.404824	0.0592216	-6.24E-05	3.70E-08	-9.34E-12	-33187.428	100.74243	-166190
1	3321164.64	-14497.179	27.084202	-0.0028793	5.56E-07	-5.73E-11	2.44E-15	65077.412	-153.62353	-166190
CH3COOH										
0	-32192.1497	1196.3196	-8.7058133	0.0569626	-5.76E-05	3.35E-08	-8.61E-12	-58401.075	72.824039	-432249.04
1	2103541.15	-14678.324	33.828159	-0.0056949	1.34E-06	-1.61E-10	7.65E-15	29242.913	-193.52882	-432249.04
C2H5										
0	-141132.838	2714.3118	-15.349908	0.0645171	-7.26E-05	4.60E-08	-1.22E-11	598.01177	109.09736	118658.24
1	4169208.95	-16629.796	27.954403	-0.0030517	5.69E-07	-5.68E-11	2.36E-15	113700.84	-163.93569	118658.24
C2H5Br										
0	-137417.2641	2861.4294	-18.241089	0.0856623	-1.05E-04	6.91E-08	-1.86E-11	-21984.802	125.84354	-63600
1	2378652.344	-12670.344	27.775594	-0.0020109	4.44E-07	-5.35E-11	2.64E-15	64140.669	-152.82778	-63600
C2H6										
0	-186205.03	3406.2007	-19.517101	0.0756585	-8.20E-05	5.06E-08	-1.32E-11	-27029.371	129.8143	-83851.544
1	5025809.41	-20330.305	33.225621	-0.0038368	7.24E-07	-7.32E-11	3.07E-15	111596.91	-203.94175	-83851.544
CH3N2CH3										
0	-373848.171	5880.4339	-29.863851	0.1087376	-1.17E-04	6.92E-08	-1.72E-11	-11899.753	194.8239	148699.36
1	4993354.46	-21609.985	39.644559	-0.0041965	8.02E-07	-8.21E-11	3.48E-15	144996.38	-237.21139	148699.36
C2H5OH										
0	-234281.0005	4479.2056	-27.448302	0.1088682	-1.31E-04	8.44E-08	-2.23E-11	-50222.412	176.48363	-234950
1	4694781.59	-19297.895	34.47576	-0.0032361	5.78E-07	-5.56E-11	2.23E-15	86015.652	-203.4796	-234950
CH3OCH3										
0	-269308.197	4300.6923	-21.527823	0.0813183	-8.30E-05	4.80E-08	-1.19E-11	-44102.281	146.76636	-184110
1	4933577.31	-20830.944	36.290524	-0.0041084	7.90E-07	-8.13E-11	3.46E-15	101330.12	-218.54482	-184110
CCN										
0	-17952.6643	144.57703	3.6136358	0.0057475	-2.88E-06	-1.70E-10	4.09E-13	94603.815	6.9578716	804803.41
1	91176.8006	-1382.9034	8.3726195	-2.69E-04	3.52E-08	-5.69E-13	-8.40E-17	102581.31	-22.784412	804803.41
CNC										
0	-70814.8772	1008.4424	-1.5790465	0.0205286	-2.28E-05	1.28E-08	-2.93E-12	76128.661	34.887809	684917.12
1	-90327.5316	-830.95294	8.1143379	-2.45E-04	5.39E-08	-6.18E-12	2.86E-16	84516.612	-21.023806	684917.12
C2N2										
0	108239.1272	-1928.1144	15.538731	-0.0182114	2.78E-05	-1.90E-08	4.95E-12	44490.887	-60.908939	309100
1	795063.152	-4001.9008	13.149756	-8.77E-04	2.07E-07	-2.21E-11	1.00E-15	58665.44	-54.766961	309100
C2O										
0	-2440.76271	-134.96366	4.7332664	0.0032998	-8.83E-08	-1.78E-09	7.83E-13	34210.613	-0.3017906	291039.37
1	325488.782	-2339.5357	9.7415954	-0.0012456	3.76E-07	-5.08E-11	2.54E-15	46600.452	-33.006893	291039.37
C3										
0	-43545.6285	666.01041	1.4510151	0.0074344	-3.81E-06	-2.34E-11	4.41E-13	96351.74	20.251418	839948.5
1	4508043.98	-14610.16	22.81947	-0.0085442	2.15E-06	-2.10E-10	6.35E-15	191196.49	-127.1855	839948.5
2	5.62E+08	-480014.82	148.7736	-0.0186381	1.25E-06	-4.23E-11	5.70E-16	3777690.2	-1226.3494	839948.5
C3H3,1-propynl										
0	-65058.5935	1350.8589	-5.8254339	0.0375661	-3.73E-05	2.12E-08	-5.14E-12	46565.105	57.814706	450000
1	4550654.87	-16405.742	27.12606	-0.0044746	1.04E-06	-1.25E-10	6.03E-15	153408.77	-156.59325	450000
C3H3,2-propynl										
0	61885.7832	-890.95787	6.3475588	0.0163317	-1.95E-05	1.42E-08	-4.20E-12	42717.858	-12.314076	331800
1	2989723.833	-11189.544	22.222251	-0.0020681	4.12E-07	-4.44E-11	1.97E-15	106187.83	-118.67453	331800
C3H4,allene										
0	-16456.1721	963.01265	-7.5327046	0.0551833	-6.73E-05	4.53E-08	-1.25E-11	17724.623	61.522156	190920
1	3479262.9	-14303.87	27.025075	-0.0025573	4.71E-07	-4.65E-11	1.91E-15	107229.59	-154.88229	190920

C3H4,propyne										
0	-35639.2347	832.81864	-4.0737806	0.0411393	-4.47E-05	2.85E-08	-7.70E-12	17055.133	45.167295	184510
1	3710430.05	-14891.429	27.323948	-0.0026453	4.86E-07	-4.79E-11	1.96E-15	110442.77	-156.79911	184510
C3H4,cyclo-										
0	-19697.998	1505.418	-14.182273	0.0764269	-9.77E-05	6.61E-08	-1.81E-11	26256.131	96.047444	277100
1	3168385.27	-13710.426	26.643032	-0.0024204	4.43E-07	-4.35E-11	1.78E-15	113368.21	-152.2619	277100
C3H5,allyl										
0	-124131.416	2245.5735	-11.778449	0.0622261	-6.76E-05	4.18E-08	-1.09E-11	8381.3241	91.069756	169000
1	3978759.95	-16874.264	31.424568	-0.0033068	6.34E-07	-6.51E-11	2.76E-15	119643.36	-181.81813	169000
C3H6,propylene										
0	-191245.297	3542.0597	-21.148696	0.0890146	-1.00E-04	6.27E-08	-1.64E-11	-15299.55	140.76361	20000
1	5017620.82	-20860.848	36.441579	-0.0038812	7.28E-07	-7.32E-11	3.05E-15	126124.58	-219.57172	20000
C3H6,cyclo-										
0	-156584.681	4111.2141	-32.334943	0.1306351	-1.65E-04	1.10E-07	-2.96E-11	-12453.12	193.15848	53300
1	4784990.8	-20421.175	36.31497	-0.0035613	6.48E-07	-6.33E-11	2.57E-15	126827.35	-222.37301	53300
C3H6O										
0	-229283.757	4495.7819	-29.411355	0.1213118	-1.44E-04	9.20E-08	-2.42E-11	-33177.124	184.6887	-93720
1	4789694.05	-21068.87	39.546388	-0.0039109	7.33E-07	-7.36E-11	3.06E-15	112033.87	-237.19987	-93720
C3H7,n-propyl										
0	-189534.427	3949.5279	-26.062221	0.1121922	-1.37E-04	9.02E-08	-2.44E-11	-7227.9282	167.37086	100500
1	5646500.41	-22910.851	39.872749	-0.0041062	7.56E-07	-7.48E-11	3.07E-15	148300.54	-240.37811	100500
C3H7,i-propyl										
0	-295208.637	5294.4659	-31.053061	0.1143877	-1.29E-04	8.06E-08	-2.09E-11	-14768.315	198.80926	93300
1	5806950.76	-24112.08	40.852784	-0.0045178	8.50E-07	-8.57E-11	3.58E-15	154649.61	-248.70912	93300
C3H8										
0	-243172.255	4653.4554	-29.373779	0.1188288	-1.38E-04	8.81E-08	-2.34E-11	-35390.841	184.06406	-104680
1	6421429.17	-26600.176	45.34513	-0.0050213	9.47E-07	-9.58E-11	4.01E-15	145572.98	-281.84937	-104680
C3H8O,1propanol										
0	-250406.391	5035.211	-32.261731	0.1345966	-1.59E-04	1.02E-07	-2.71E-11	-55368.752	204.18423	-255200
1	5460837.77	-23961.172	44.598163	-0.0033846	5.40E-07	-4.65E-11	1.64E-15	109718.82	-267.39691	-255200
C3H8O,2propanol										
0	-338872.14	6109.3847	-37.933374	0.153099	-1.86E-04	1.21E-07	-3.22E-11	-62815.354	233.53868	-272700
1	6000115.5	-25056.237	46.219282	-0.0042718	7.69E-07	-7.45E-11	3.00E-15	114835	-279.60046	-272700
C3O2										
0	157980.197	-2529.381	18.016917	-0.0178581	2.98E-05	-2.18E-08	6.01E-12	-1121.8217	-72.773426	-93640
1	696713.757	-4624.3152	16.638625	-0.0011753	2.48E-07	-2.74E-11	1.24E-15	12522.857	-72.756573	-93640
C4										
0	39031.8911	-894.73978	10.509016	-0.0065514	1.24E-05	-8.64E-09	2.26E-12	126642.17	-30.77315	1033903.7
1	920096.292	-1530.4025	6.0501845	0.0052527	-1.78E-06	2.59E-10	-1.39E-14	133439.53	-7.2619982	1033903.7
C4H2										
0	246751.587	-3897.8172	23.66059	-0.0220802	2.78E-05	-1.58E-08	3.42E-12	70868.894	-110.9162	450000
1	2328169.46	-8925.163	21.143255	-0.0013689	2.33E-07	-2.12E-11	8.05E-16	105778.69	-108.83128	450000
C4H4,1,3-cyclo-										
0	-27785.0285	1768.1869	-17.579002	0.0938352	-1.20E-04	7.98E-08	-2.15E-11	38116.223	112.84806	385000
1	2991530.65	-14167.93	30.019941	-0.0025793	4.79E-07	-4.78E-11	1.98E-15	127467.41	-172.75431	385000
C4H6,butadiene										
0	-91811.2969	3312.5704	-29.858286	0.1479201	-2.06E-04	1.47E-07	-4.15E-11	-2077.309	178.06866	110000
1	-2.36E+07	56513.241	-32.75739	0.0229307	-2.30E-06	4.29E-11	4.24E-15	-367135.91	301.34371	110000
C4H6,1-butyne										
0	-55970.396	1433.1917	-9.6912105	0.0715	-8.16E-05	5.29E-08	-1.44E-11	11849.87	76.602186	165200
1	4032213.88	-19072.555	38.325732	-0.0039413	9.17E-07	-1.13E-10	5.66E-15	130173.34	-225.27405	165200
C4H6,2-butyne										
0	-265075.642	4490.7287	-24.007239	0.0981958	-1.08E-04	6.68E-08	-1.74E-11	-5328.3638	159.50346	145700
1	3790405.23	-18216.269	36.039873	-0.0021452	3.53E-07	-3.22E-11	1.25E-15	122811.96	-211.8773	145700
C4H6,cyclo-										
0	-204673.149	4919.504	-37.532965	0.1497298	-1.86E-04	1.22E-07	-3.25E-11	-3916.1114	223.3292	156700
1	4517319.22	-20973.021	40.080327	-0.0039498	7.45E-07	-7.53E-11	3.15E-15	140646.31	-243.48322	156700
C4H8,1-butene										
0	-272149.18	5100.079	-31.837861	0.1317754	-1.53E-04	9.71E-08	-2.56E-11	-25230.963	200.69314	-540
1	1.25E+07	-45237.714	69.096747	-0.016345	4.08E-06	-5.10E-10	2.50E-14	275371.53	-444.64849	-540
C4H8,cis2-buten										
0	-277387.055	5382.3836	-33.751879	0.1322981	-1.49E-04	9.28E-08	-2.41E-11	-27158.841	211.44613	-7400
1	1.20E+07	-44145.038	67.355102	-0.0152266	3.74E-06	-4.62E-10	2.24E-14	267404.35	-434.22339	-7400
C4H8,tr2-butene										
0	-359464.4	5930.9719	-32.558252	0.1254958	-1.37E-04	8.41E-08	-2.16E-11	-31132.965	207.00805	-11000
1	1.33E+07	-48349.179	72.864678	-0.0185507	4.74E-06	-6.05E-10	3.02E-14	293563.78	-472.90211	-11000
C4H8,isobutene										
0	-232720.493	3941.994	-22.245811	0.1012791	-1.07E-04	6.45E-08	-1.65E-11	-22337.66	147.95969	-17100
1	1.48E+07	-52349.083	77.470025	-0.0212175	5.53E-06	-7.17E-10	3.63E-14	318424.11	-505.95051	-17100
C4H8,cyclo-										
0	-304765.582	6519.4825	-46.629875	0.1743593	-2.09E-04	1.34E-07	-3.54E-11	-27000.311	273.83475	28400
1	4456210.65	-23010.177	44.924477	-0.0030801	5.32E-07	-5.08E-11	2.05E-15	135548.71	-277.18021	28400
(CH3COOH)2										
0	-309478.797	5983.485	-35.730589	0.1662537	-1.88E-04	1.15E-07	-2.94E-11	-142150.08	229.58879	-929015.36
1	6571343.94	-30368.779	62.50391	-0.0057327	1.08E-06	-1.10E-10	4.61E-15	63474.7	-373.45649	-929015.36
C4H9,n-butyl										
0	-223956.041	4676.5541	-29.854245	0.1345494	-1.60E-04	1.05E-07	-2.81E-11	-15252.977	190.16509	66530
1	1.26E+07	-45720.902	70.995022	-0.0158093	3.91E-06	-4.86E-10	2.37E-14	285968.97	-454.14007	66530
C4H9,i-butyl										
0	-239946.123	4697.4445	-30.874725	0.1391656	-1.67E-04	1.09E-07	-2.94E-11	-16381.51	193.66617	57320
1	8297503.79	-32966.211	56.628692	-0.0078496	1.67E-06	-1.84E-10	8.22E-15	203582.61	-352.37992	57320
C4H9,s-butyl										

0	-335105.033	6312.9281	-40.030152	0.1563872	-1.84E-04	1.18E-07	-3.13E-11	-22160.371	248.12898	71000
1	7224663.58	-30352.724	52.885368	-0.005652	1.06E-06	-1.07E-10	4.44E-15	188348.18	-325.57088	71000
C4H9,t-butyl										
0	-472347.963	8090.2278	-46.836939	0.1575306	-1.69E-04	9.98E-08	-2.49E-11	-33193.809	289.48485	51700
1	7150931.1	-31711.884	54.424731	-0.0063921	1.24E-06	-1.29E-10	5.51E-15	193448.37	-339.92986	51700
C4H10,isobutane										
0	-383447.954	7000.0491	-44.400288	0.1746183	-2.08E-04	1.34E-07	-3.55E-11	-50340.24	265.89676	-134990
1	7527789.56	-32024.574	57.001012	-0.0060597	1.14E-06	-1.16E-10	4.85E-15	172846.2	-357.61337	-134990
C4H10,n-butane										
0	-317578.326	6176.1597	-38.914286	0.1584612	-1.86E-04	1.20E-07	-3.20E-11	-45402.881	237.94175	-125790
1	7682227.69	-32560.269	57.367004	-0.0061977	1.18E-06	-1.22E-10	5.25E-15	177451.1	-358.78962	-125790
C4N2										
0	148921.395	-2815.8267	22.435837	-0.0237505	3.84E-05	-2.74E-08	7.37E-12	74780.976	-95.941648	533460
1	1026263.52	-5887.5619	20.456103	-0.00147	3.08E-07	-3.40E-11	1.53E-15	95047.298	-95.413209	533460
C5										
0	-12011.3532	-555.32181	11.23801	-0.0043471	1.74E-05	-1.71E-08	5.57E-12	126240.23	-32.621613	1050924.3
1	217246.948	-2958.6578	15.610995	-8.20E-04	1.78E-07	-2.01E-11	9.22E-16	139521.73	-64.332128	1050924.3
C5H6,1,3cyclo-										
0	-101669.408	3484.8187	-31.878878	0.1472154	-1.85E-04	1.23E-07	-3.29E-11	329.24556	189.05313	134300
1	4448856.56	-21284.436	43.144087	-0.0039363	7.36E-07	-7.39E-11	3.08E-15	138575.89	-260.93283	134300
C5H8,cyclo-										
0	-263111.442	5987.7532	-45.222445	0.1804626	-2.18E-04	1.40E-07	-3.70E-11	-23795.046	266.01357	33900
1	4569864.86	-24060.225	48.810105	-0.0034131	6.05E-07	-5.93E-11	2.45E-15	141398.59	-298.95372	33900
C5H10,1-pentene										
0	-534054.793	9298.9171	-56.677923	0.21231	-2.57E-04	1.67E-07	-4.43E-11	-47906.82	339.60357	-21280
1	4536789.7	-24837.752	53.161381	-0.0041222	9.90E-07	-1.25E-10	6.29E-15	138141.29	-318.85242	-21280
C5H10,cyclo-										
0	-414112.487	8627.5976	-62.029612	0.2259911	-2.68E-04	1.71E-07	-4.46E-11	-49471.6	358.39167	-78400
1	7501820.61	-35058.344	63.2245	-0.0069402	1.34E-06	-1.38E-10	5.87E-15	195334.22	-402.65289	-78400
C5H11,pentyl										
0	-465371.588	8564.2205	-52.952429	0.2094289	-2.56E-04	1.69E-07	-4.60E-11	-36417.043	319.68616	45810
1	1.25E+07	-49272.359	81.657979	-0.0168141	4.20E-06	-5.22E-10	2.55E-14	300998.68	-520.38098	45810
C5H11,t-pentyl										
0	-515219.716	9144.3542	-56.024157	0.199821	-2.24E-04	1.38E-07	-3.52E-11	-40362.787	340.28202	32600
1	8601872.9	-38051.438	66.49628	-0.0075336	1.45E-06	-1.50E-10	6.37E-15	228181.86	-416.93635	32600
C5H12,n-pentane										
0	-332492.538	6564.5071	-39.823786	0.1623257	-1.65E-04	8.97E-08	-1.99E-11	-50223.079	247.2553	-146760
1	6212257.35	-32125.785	64.063534	-0.0053071	1.15E-06	-1.35E-10	6.54E-15	166725.26	-396.08584	-146760
C5H12,i-pentane										
0	-423190.329	6497.189	-36.811269	0.1532425	-1.55E-04	8.75E-08	-2.07E-11	-51554.166	230.95176	-153700
1	8502517.22	-37111.428	66.381394	-0.0038697	5.64E-07	-4.86E-11	1.87E-15	199903.84	-417.62711	-153700
CH3C(CH3)2CH3										
0	-8973221.99	128922.56	-719.93446	2.0568621	-0.0029532	2.16E-06	-6.27E-10	-639493.18	4020.8062	-167920
1	1.68E+07	-59794.892	86.855069	-0.0096222	1.65E-06	-1.67E-10	7.37E-15	345853.52	-576.05082	-167920
C6H2										
0	290381.704	-4929.8831	31.893944	-0.0311964	4.33E-05	-2.73E-08	6.68E-12	101190.5	-153.06331	670000
1	2592801.45	-10833.516	28.47452	-0.0018767	3.41E-07	-3.34E-11	1.36E-15	141851.03	-149.48481	670000
C6H5,phenyl										
0	-160234.195	3937.4893	-32.003276	0.1437286	-1.74E-04	1.11E-07	-2.89E-11	22071.064	193.3059	337200
1	3767622.46	-19531.258	42.274244	-0.0036985	7.00E-07	-7.11E-11	2.99E-15	151244.13	-251.51033	337200
C6D5,phenyl										
0	0	0	-1.2549782	0.0473288	-8.08E-06	-2.99E-08	1.71E-11	35314.063	29.78008	306947.83
1	0	0	14.729492	0.0152105	-5.52E-06	8.80E-10	-5.10E-14	30282.629	-55.75503	306947.83
C6H5O,phenoxy										
0	-129226.781	3406.7454	-29.113696	0.1459181	-1.78E-04	1.14E-07	-2.97E-11	-10550.579	177.0683	47697.6
1	3678627.4	-19729.785	45.411833	-0.0037511	7.11E-07	-7.23E-11	3.05E-15	116359.15	-268.10579	47697.6
C6H6										
0	-168282.654	4412.5145	-37.220639	0.1641918	-2.02E-04	1.31E-07	-3.45E-11	-10392.543	217.24421	82880
1	4549770.27	-22615.339	46.922072	-0.0041968	7.87E-07	-7.92E-11	3.30E-15	139238.84	-286.76898	82880
C6D6										
0	0	0	-2.0701218	0.0529382	-9.61E-06	-3.28E-08	1.90E-11	5406.8984	30.693809	58177.984
1	0	0	15.619864	0.0171239	-6.20E-06	9.85E-10	-5.69E-14	-144.33052	-63.888253	58177.984
C6H5OH,phenol										
0	-120948.716	3378.4132	-29.919279	0.1567827	-1.97E-04	1.29E-07	-3.42E-11	-27794.421	179.97528	-96399
1	4462031.21	-21655.079	48.150057	-0.0035682	6.33E-07	-6.04E-11	2.40E-15	111371.75	-286.04477	-96399
C6H10,cyclo-										
0	-375031.308	7643.9119	-55.104484	0.2166233	-2.55E-04	1.61E-07	-4.19E-11	-36610.908	320.24173	-4600
1	7510055.18	-35568.376	67.030128	-0.0070452	1.36E-06	-1.40E-10	5.96E-15	206026.11	-423.8182	-4600
C6H12,1-hexene										
0	-669250.578	11802.327	-72.895473	0.2714479	-3.34E-04	2.19E-07	-5.87E-11	-62319.405	429.71571	-41950
1	5055636.74	-27978.969	61.934186	-0.0042981	1.06E-06	-1.35E-10	6.86E-15	152516.07	-372.10897	-41950
C6H12,cyclo-										
0	-568004.3	10342.456	-68.000725	0.2387804	-2.51E-04	1.43E-07	-3.41E-11	-64046.694	393.4826	-123300
1	5224978.7	-33641.535	71.745697	-0.0066988	1.32E-06	-1.39E-10	6.06E-15	173251.06	-454.67867	-123300
C6H13,n-hexyl										
0	-1427278.21	22488.281	-129.74922	0.4279797	-5.56E-04	3.79E-07	-1.05E-10	-106026.1	749.71861	25100
1	1.34E+07	-55710.558	95.520218	-0.0196212	5.02E-06	-6.38E-10	3.18E-14	334575.61	-609.5259	25100
C6H14,n-hexane										
0	-581592.654	10790.977	-66.339469	0.2523715	-2.90E-04	1.80E-07	-4.62E-11	-72715.445	393.82829	-166920
1	1.80E+07	-66812.212	106.27819	-0.0226096	5.74E-06	-7.35E-10	3.71E-14	384032.66	-691.24548	-166920
C7H7,benzyl										
0	-183673.533	4102.4154	-32.02373	0.1588239	-1.89E-04	1.20E-07	-3.14E-11	5266.5651	193.87335	210500

1	5297206.15	-25998.793	55.097208	-0.0049775	9.46E-07	-9.64E-11	4.06E-15	173836.33	-334.3808	210500
C7H8										
0	-287803.695	6134.0474	-45.747652	0.1936912	-2.30E-04	1.46E-07	-3.79E-11	-23084.533	269.39472	50170
1	6184514.65	-29902.798	59.820038	-0.005697	1.08E-06	-1.10E-10	4.62E-15	178204.49	-369.80808	50170
C7H8O,cresol-mx										
0	-244392.253	5084.3038	-37.905533	0.1865208	-2.27E-04	1.46E-07	-3.82E-11	-40953.435	228.22501	-132298
1	6017427.26	-28499.615	60.815966	-0.004997	9.13E-07	-8.98E-11	3.67E-15	147226.5	-367.48913	-132298
C7H14,1-heptene										
0	-747715.05	13361.271	-83.034337	0.3114021	-3.80E-04	2.45E-07	-6.51E-11	-72368.252	486.87802	-62760
1	5164927.02	-29882.004	69.269669	-0.0036731	9.17E-07	-1.17E-10	5.92E-15	159015.59	-415.09951	-62760
C7H15,n-heptyl										
0	-1671733.52	26400.103	-152.68677	0.5027121	-6.52E-04	4.44E-07	-1.23E-10	-127375.46	878.39327	4390
1	1.40E+07	-60952.08	107.52726	-0.0211597	5.41E-06	-6.88E-10	3.43E-14	360996.45	-685.83821	4390
C7H16,2-methylh										
0	-710477.795	11912.511	-73.453396	0.2902952	-3.46E-04	2.26E-07	-6.13E-11	-82021.478	432.00417	-194600
1	1.28E+07	-55708.389	100.0868	-0.0135681	3.28E-06	-4.15E-10	2.10E-14	304812.13	-638.40292	-194600
C7H16,n-heptane										
0	-612743.275	11840.854	-74.871884	0.2918466	-3.42E-04	2.16E-07	-5.66E-11	-80134.088	440.72126	-187780
1	1.28E+07	-54125.621	98.011946	-0.0138271	3.43E-06	-4.36E-10	2.20E-14	296664.87	-621.67644	-187780
C8H8,styrene										
0	-268693.04	6167.9993	-48.360548	0.2182873	-2.74E-04	1.81E-07	-4.87E-11	-11406.399	281.76783	148300
1	1638245.27	-20099.574	55.943421	-0.0040595	1.00E-06	-1.30E-10	6.75E-15	122748.46	-330.92622	148300
C8H10,ethylbenz										
0	-469493.99	9307.168	-65.217693	0.261208	-3.18E-04	2.05E-07	-5.40E-11	-40738.701	378.09036	29920
1	5206906.88	-30750.408	68.231595	-0.0061464	1.39E-06	-1.66E-10	8.09E-15	175873.13	-418.46319	29920
C8H16,1-octene										
0	-931388.193	16455.233	-101.84448	0.3754864	-4.60E-04	2.97E-07	-7.86E-11	-89742.532	592.15488	-83590
1	5983719.61	-33433.251	78.085943	-0.003725	9.35E-07	-1.19E-10	5.97E-15	176415.13	-469.01491	-83590
C8H17,n-octyl										
0	-1934340.97	30549.798	-176.79034	0.5801597	-7.52E-04	5.11E-07	-1.41E-10	-149889.47	1013.7243	-16320
1	1.49E+07	-66587.393	119.93214	-0.0228938	5.86E-06	-7.45E-10	3.70E-14	389971.07	-765.04451	-16320
C8H18,n-octane										
0	-698664.724	13385.011	-84.151661	0.3271937	-3.78E-04	2.34E-07	-6.01E-11	-90262.234	493.92221	-208750
1	7872500.12	-42644.156	92.143265	-0.0070119	1.73E-06	-2.21E-10	1.12E-14	216195.34	-568.10637	-208750
C8H18,isooctane										
0	-168875.867	3126.9034	-21.235029	0.1489152	-1.15E-04	4.47E-08	-5.55E-12	-44680.607	141.74552	-224010
1	2.54E+07	-91319.306	138.71548	-0.0227382	5.27E-06	-6.58E-10	3.31E-14	529263.83	-919.63076	-224010
C9H19,n-nonyl										
0	-2194880.61	34685.658	-200.92614	0.6580503	-8.53E-04	5.79E-07	-1.60E-10	-172319.46	1149.114	-37030
1	1.56E+07	-72063.779	132.17221	-0.0245443	6.28E-06	-7.98E-10	3.97E-14	417919.33	-843.05702	-37030
C10H8,naphthale										
0	-260292.099	6237.5193	-52.261574	0.2397711	-2.91E-04	1.85E-07	-4.82E-11	-11147.533	297.21727	150580
1	5905864.57	-31631.449	70.302526	-0.0060184	1.14E-06	-1.16E-10	4.89E-15	196251.27	-434.77857	150580
C10H21,n-decyl										
0	-2446511.14	38700.813	-224.43882	0.7343625	-9.51E-04	6.46E-07	-1.78E-10	-194163.39	1280.9878	-57740
1	1.65E+07	-77792.223	144.68424	-0.0263357	6.75E-06	-8.56E-10	4.25E-14	447483.24	-923.03234	-57740
C12H9,o-bipheny										
0	-359593.888	7661.5434	-58.733895	0.2697584	-3.23E-04	2.03E-07	-5.23E-11	14583.42	339.27421	427730.32
1	6736160.26	-36321.145	82.101574	-0.0075019	1.46E-06	-1.51E-10	6.44E-15	255547.3	-504.24038	427730.32
C12D9,o-bipheny										
0	0	0	-0.732994	0.0898369	-1.37E-05	-5.94E-08	3.37E-11	42943.094	30.041889	386511.72
1	0	0	30.123199	0.0283283	-1.04E-05	1.66E-09	-9.65E-14	33207.789	-135.19137	386511.72
C12H10,biphenyl										
0	-367113.641	8128.5828	-63.910961	0.2901449	-3.51E-04	2.23E-07	-5.79E-11	-16793.423	363.35206	182130
1	7480124.81	-39280.195	86.614115	-0.007946	1.53E-06	-1.58E-10	6.70E-15	243800.67	-538.13307	182130
C12D10,biphenyl										
0	0	0	-1.5793486	0.0950596	-1.45E-05	-6.26E-08	3.55E-11	13137.422	31.529775	138415.82
1	0	0	30.90506	0.03035	-1.11E-05	1.78E-09	-1.03E-13	2883.4453	-142.439	138415.82
Ca										
0	0	0	2.5	0	0	0	0	20638.928	4.3845483	177800
1	7547341.24	-21486.427	25.308496	-0.0110377	2.29E-06	-1.21E-10	-4.02E-15	158586.23	-160.9513	177800
2	2.29E+09	-1608863	431.24664	-0.0539651	3.53E-06	-1.16E-10	1.53E-15	1.26E+07	-3692.1016	177800
Ca+										
0	0	0	2.5	0	0	0	0	92324.178	5.077675	773827.73
1	3747070.82	-11747.077	16.72547	-0.0083348	2.39E-06	-2.99E-10	1.36E-14	166432.91	-95.828213	773827.73
2	9.12E+08	-622042.85	168.37411	-0.0214086	1.45E-06	-4.92E-11	6.58E-16	4959472.1	-1422.6007	773827.73
CaBr										
0	569.383262	-125.75135	5.0015083	-0.0010399	1.38E-06	-8.95E-10	2.40E-13	-3728.104	1.7848648	-24868.681
1	2783236.402	-8458.2037	14.317566	-0.0054308	1.52E-06	-1.83E-10	7.86E-15	49312.707	-65.370011	-24868.681
CaBr2										
0	1572.504318	-223.85512	8.3884579	-0.0019442	2.40E-06	-1.56E-09	4.12E-13	-47721.066	-10.749652	-387197.3
1	-22198.46426	-4.4631553	7.5037551	-1.64E-06	3.88E-10	-4.68E-14	2.26E-18	-48854.368	-5.5903243	-387197.3
CaCL										
0	6395.33526	-224.90423	5.2832784	-0.001448	1.64E-06	-9.43E-10	2.24E-13	-12701.69	-1.3919702	-103772.89
1	1629182.545	-4766.223	9.6589298	-0.002523	5.83E-07	-4.10E-11	8.81E-17	16625.992	-33.987318	-103772.89
CaCL+										
0	2285.284542	-200.28727	4.9369902	-3.86E-04	8.69E-08	1.47E-10	-7.69E-14	55882.78	-0.6359875	467190.51
1	177028.0396	-589.13724	5.1033688	-2.36E-04	5.48E-08	2.14E-14	-5.57E-16	58534.173	-2.1912596	467190.51
CaCL2										
0	11068.0203	-424.91083	9.1347119	-0.0034972	4.24E-06	-2.72E-09	7.14E-13	-58503.468	-18.086791	-485243.48
1	-35957.6878	-8.7964956	7.5072569	-3.13E-06	7.32E-10	-8.78E-14	4.21E-18	-60667.797	-8.5535316	-485243.48
CaF										

0	31842.354	-491.82351	5.7011209	-0.0014651	9.09E-07	-1.37E-10	-5.11E-14	-31976.941	-5.9966623	-276403.79
1	519588.267	-1512.3216	5.8692763	-3.88E-04	-2.48E-08	3.75E-11	-3.47E-15	-24888.146	-8.6146637	-276403.79
CaF+										
0	41583.408	-562.76617	5.6875222	-0.0012647	6.67E-07	-6.93E-11	-3.98E-14	33051.195	-6.974485	260664.61
1	-139867.0845	219.15264	4.2143243	2.14E-04	-5.78E-08	9.99E-12	-6.06E-16	28416.059	2.7403427	260664.61
CaF2										
0	59093.5229	-1019.733	10.131653	-0.0055035	5.63E-06	-3.12E-09	7.21E-13	-91926.082	-26.39506	-790828.41
1	-82804.0944	-31.159501	7.0235774	-9.52E-06	2.12E-09	-2.44E-13	1.14E-17	-97294.668	-7.5462433	-790828.41
CaH										
0	-45137.8223	762.94292	-1.2808742	0.0131877	-1.48E-05	8.54E-09	-1.99E-12	23003.788	30.534215	229409.11
1	-2696952.529	8607.0598	-7.0274548	0.0074679	-2.32E-06	3.42E-10	-1.89E-14	-27738.191	78.45822	229409.11
CaI										
0	-826.179018	-85.089759	4.8641717	-7.86E-04	1.10E-06	-7.35E-10	2.01E-13	523.67534	3.5853917	12183.32
1	1771071.309	-5683.6437	11.538575	-0.004194	1.29E-06	-1.73E-10	8.38E-15	35832.932	-44.059176	12183.32
CaI2										
0	-1097.851401	-145.98218	8.0893418	-0.0013053	1.62E-06	-1.06E-09	2.83E-13	-32726.93	-6.9817149	-259319.51
1	-16237.27104	-2.8595307	7.5024322	-1.07E-06	2.54E-10	-3.08E-14	1.49E-18	-33463.412	-3.5673057	-259319.51
CaO										
0	38897.3307	-483.56774	5.0777133	3.08E-04	-1.16E-06	8.49E-10	-1.50E-13	5937.6435	-3.9553207	38005.308
1	-4.91E+07	149586.6	-168.16541	0.0938195	-2.46E-05	3.07E-09	-1.49E-13	-946151.17	1235.6948	38005.308
2	-3.50E+08	208321.24	-39.782093	0.0050393	-3.22E-07	1.06E-11	-1.40E-16	-1662378.7	393.44919	38005.308
CaO+										
0	109806.0332	-1459.9924	9.8807779	-0.0091576	8.71E-06	-4.39E-09	9.26E-13	91500.574	-30.099477	710237.54
1	939784.313	-2993.3622	8.3361918	-0.0023033	7.37E-07	-1.05E-10	5.26E-15	102809.84	-24.615478	710237.54
2	-7.65E+07	17392.453	8.4202887	-0.0011684	8.41E-08	-2.77E-12	3.57E-17	-86434.898	-23.765131	710237.54
CaOH										
0	46200.289	-928.56728	9.1758288	-0.0039628	2.51E-06	3.85E-11	-3.35E-13	-17980.097	-25.337049	-173307.35
1	1979972.994	-5598.881	11.513487	-0.0016683	3.31E-07	-1.79E-11	-3.58E-16	13401.968	-46.460843	-173307.35
CaOH+										
0	48843.4266	-983.24151	9.610183	-0.0052044	4.26E-06	-1.20E-09	9.03E-15	47950.563	-28.270773	372938.1
1	863761.537	-2347.302	7.9819112	1.00E-04	-6.24E-08	1.02E-11	-5.70E-16	58305.801	-21.521819	372938.1
Ca(OH)2										
0	83892.5754	-1791.9021	16.21891	-0.0078409	5.10E-06	-6.96E-11	-6.13E-13	-66004.056	-60.709139	-598338.87
1	1721854.884	-4702.2177	13.969477	1.98E-04	-1.24E-07	2.03E-11	-1.14E-15	-44437.614	-52.874449	-598338.87
CaS										
0	23209.90615	-451.84461	6.1723338	-0.0035989	4.82E-06	-3.63E-09	1.21E-12	15545.977	-7.6869157	121475.31
1	-1.57E+07	52938.558	-63.224672	0.0402773	-1.11E-05	1.46E-09	-7.38E-14	-317202.27	479.96062	121475.31
Ca2										
0	-85822.2862	158.8189	11.039521	-0.033332	5.35E-05	-4.01E-08	1.16E-11	37703.508	-23.977446	341765.34
1	240596.6267	57.758038	2.3474367	1.20E-04	-4.33E-08	7.02E-12	-3.71E-16	40818.754	18.953996	341765.34
Cd										
0	-1.08E-04	1.82E-06	2.5	3.13E-11	-4.60E-14	3.41E-17	-9.99E-21	12700.998	5.9315498	111800
1	-269975.7467	786.60011	1.6281691	4.59E-04	-1.15E-07	1.07E-11	8.79E-17	7675.1483	12.200061	111800
2	-1.34E+09	932094.91	-249.09562	0.0330288	-2.20E-06	7.43E-11	-1.03E-15	-7267529	2167.9461	111800
Cd+										
0	4.10E-04	-4.34E-06	2.5	-4.39E-11	5.56E-14	-3.64E-17	9.61E-21	117812.94	6.6246895	985754.33
1	14848.80812	-46.691537	2.557883	-3.62E-05	1.21E-08	-2.07E-12	1.42E-16	118107.01	6.2164145	985754.33
2	-6.43E+07	47403.952	-11.657555	0.0022203	-1.96E-07	9.26E-12	-1.56E-16	-248924.45	126.39463	985754.33
CL										
0	22762.15854	-216.84133	2.7451851	0.0024511	-5.46E-06	4.42E-09	-1.29E-12	15013.571	3.1029508	121301
1	-169793.293	608.17265	2.1286641	1.31E-04	-2.64E-08	2.84E-12	-1.25E-16	9934.3874	8.8447594	121301
2	-7.14E+07	44999.363	-9.2643154	0.0016574	-1.33E-07	5.53E-12	-8.39E-17	-340533.3	106.91113	121301
CL+										
0	103469.7859	-1293.7589	8.1867027	-0.009916	9.21E-06	-4.51E-09	9.18E-13	171475.88	-27.664192	1378799.6
1	40564.0948	-49.601657	3.1016536	-5.87E-04	2.25E-07	-3.30E-11	1.71E-15	165298.23	2.5749299	1378799.6
2	-3078099.946	-685.84183	3.0922893	-1.92E-05	3.81E-10	-1.57E-13	8.44E-18	168343.44	1.3343945	1378799.6
CL-										
0	0	0	2.5	0	0	0	0	-28883.891	4.2006293	-233957.97
1	0	0	2.5	0	0	0	0	-28883.891	4.2006293	-233957.97
2	0	0	2.5	0	0	0	0	-28883.891	4.2006293	-233957.97
CLCN										
0	72740.4343	-1297.3449	11.076765	-0.0110843	1.61E-05	-1.09E-08	2.83E-12	20843.89	-35.973707	134200
1	346757.312	-1957.8574	8.8078062	-4.39E-04	1.02E-07	-1.11E-11	4.99E-16	25819.239	-26.36886	134200
CLF										
0	33522.1081	-368.83119	4.2722886	0.0025494	-4.46E-06	3.41E-09	-9.84E-13	-5839.3697	0.2317932	-55700.993
1	3045867.173	-9979.3283	16.841623	-0.0074659	2.34E-06	-3.37E-10	1.76E-14	54471.208	-87.079879	-55700.993
CLF3										
0	128517.5171	-2140.4457	14.930965	-0.0060425	3.72E-06	-8.05E-10	-7.99E-14	-11384.596	-55.948388	-164600
1	-229495.6235	-122.0741	10.091246	-3.65E-05	8.06E-09	-9.23E-13	4.27E-17	-22828.404	-25.11606	-164600
CLF5										
0	245968.977	-4315.3321	27.269999	-0.0167019	1.42E-05	-6.43E-09	1.18E-12	-10714.318	-126.74632	-238000
1	-426936.697	-205.78405	16.154616	-6.21E-05	1.38E-08	-1.58E-12	7.33E-17	-33614.794	-57.575066	-238000
CLO										
0	-16872.68145	257.38122	2.1758461	0.0064321	-8.57E-06	5.76E-09	-1.55E-12	9829.519	13.860096	101621.12
1	409376.052	-1765.9851	7.0879006	-0.0018285	7.10E-07	-1.21E-10	7.08E-15	21518.918	-16.686464	101621.12
CLO2										
0	-11272.77696	390.3032	-0.3843019	0.0210868	-2.79E-05	1.84E-08	-4.84E-12	9756.9337	29.13262	105000
1	-163379.3802	-316.14807	7.0097873	2.84E-04	-1.18E-07	2.92E-11	-2.02E-15	11849.465	-10.911695	105000
CL2										
0	34628.1724	-554.71295	6.207591	-0.0029896	3.17E-06	-1.79E-09	4.26E-13	1534.0708	-9.438353	0
1	6092566.75	-19496.269	28.545349	-0.0144997	4.46E-06	-6.36E-10	3.33E-14	121211.72	-169.07783	0
CL2O										

0	77988.554	-1182.5379	9.5265147	-0.0025962	8.70E-07	4.48E-10	-3.04E-13	13767.296	-24.846918	79000
1	-127174.3461	-67.419632	7.0500225	-1.99E-05	4.37E-09	-4.98E-13	2.30E-17	7387.2893	-8.7974876	79000
Co										
0	-2598.939184	246.19898	-0.6106058	0.0139301	-2.21E-05	1.62E-08	-4.53E-12	49846.138	22.575842	428441.6
1	1381841.305	-3756.0367	6.6571307	-0.0012692	1.46E-07	6.57E-12	-1.10E-15	74944.429	-22.585008	428441.6
2	-5.47E+08	403770.5	-114.24132	0.0166301	-1.16E-06	3.86E-11	-5.00E-16	-3076031.8	1003.0286	428441.6
Co+										
0	102849.416	-874.47313	4.2795003	0.0022259	-7.46E-06	7.28E-09	-2.35E-12	147489.6	-5.6790192	1193003.3
1	2907386.174	-8619.7058	11.881349	-0.0035106	5.75E-07	-2.53E-11	2.98E-16	197741.92	-60.965334	1193003.3
2	2.70E+09	-1604232.1	368.73148	-0.0404115	2.37E-06	-7.12E-11	8.64E-16	1.29E+07	-3201.6625	1193003.3
Co-										
0	34594.9376	-135.50417	1.1163309	0.0090428	-1.45E-05	9.99E-09	-2.60E-12	43370.378	12.70495	358414.37
1	-574139.417	1763.1092	1.415562	3.78E-04	-7.53E-08	8.00E-12	-3.49E-16	30834.931	16.343604	358414.37
2	-712179.584	796.24471	2.3288708	1.92E-05	-1.18E-09	3.76E-14	-4.88E-19	36892.851	9.5112827	358414.37
Cr										
0	1335.658217	-21.02424	2.6319082	-4.25E-04	7.44E-07	-6.76E-10	2.51E-13	47158.666	6.0054255	397480
1	-1.12E+07	34011.637	-36.570622	0.021103	-5.52E-06	7.17E-10	-3.51E-14	-168899.34	286.44813	397480
2	3.90E+09	-2462918.5	591.56326	-0.0669712	3.95E-06	-1.17E-10	1.37E-15	1.96E+07	-5133.5106	397480
Cr+										
0	181.9187467	-2.1888435	2.5106765	-2.71E-05	3.77E-08	-2.74E-11	8.12E-15	126338.08	6.5062762	1056546.7
1	3342330.79	-10642.611	15.578843	-0.007709	2.16E-06	-2.37E-10	8.95E-15	193299.77	-86.043567	1056546.7
2	4.85E+08	-411453.58	124.28989	-0.016101	1.15E-06	-4.10E-11	5.73E-16	3281645.8	-1034.7236	1056546.7
Cr-										
0	0	0	2.5	0	0	0	0	38586.279	6.5668354	327023.43
1	0	0	2.5	0	0	0	0	38586.279	6.5668354	327023.43
2	0	0	2.5	0	0	0	0	38586.279	6.5668354	327023.43
CrN										
0	0	0	2.9304636	0.0030377	-1.27E-06	-1.18E-09	8.56E-13	59744.203	10.191881	505021.51
1	0	0	3.8649602	8.52E-04	-4.41E-07	1.07E-10	-8.37E-15	59477.437	5.2950676	505021.51
CrO										
0	0	0	2.8414996	0.0040953	-3.58E-06	8.17E-10	2.41E-13	21646.067	11.517992	188285.45
1	0	0	4.0139818	6.27E-04	-2.80E-07	6.00E-11	-4.41E-15	21346.693	5.5517151	188285.45
CrO2										
0	0	0	3.3012645	0.0081626	-5.89E-06	1.62E-11	1.08E-12	-10353.569	11.399114	-75312.81
1	0	0	5.8499998	0.0012725	-5.49E-07	1.05E-10	-7.40E-15	-11042.183	-1.7449763	-75312.81
CrO3										
0	0	0	1.9072858	0.0230496	-2.65E-05	1.29E-08	-1.84E-12	-36608.68	15.345142	-292879.66
1	0	0	8.1628946	0.0020451	-8.86E-07	1.70E-10	-1.20E-14	-38092.557	-15.895895	-292879.66
Cs										
0	54.6658407	-0.8279346	2.5049422	-1.49E-05	2.43E-08	-2.01E-11	6.70E-15	8459.3214	6.8488258	76500
1	6166040.9	-18961.755	24.832299	-0.0125198	3.31E-06	-3.35E-10	9.63E-15	128511.12	-152.29422	76500
2	-9.57E+08	432169.04	-63.71801	0.0052463	-2.37E-07	5.85E-12	-6.17E-17	-3585268.8	615.66182	76500
Cs+										
0	0	0	2.5	0	0	0	0	54387.378	6.182758	458401.83
1	0	0	2.5	0	0	0	0	54387.378	6.182758	458401.83
2	-2.48E+08	140511.55	-28.050274	0.0030879	-1.27E-07	-3.75E-13	1.21E-16	-1072498	275.68273	458401.83
Cs-										
0	0	0	2.5	0	0	0	0	2237.029	6.1827704	24797.228
1	0	0	2.5	0	0	0	0	2237.029	6.1827704	24797.228
2	0	0	2.5	0	0	0	0	2237.029	6.1827704	24797.228
CsCL										
0	0	0	4.182303	0.001376	-2.06E-06	1.48E-09	-3.98E-13	-30177.927	6.6384882	-240166.79
1	0	0	4.4798455	1.09E-04	-4.00E-09	2.06E-13	2.22E-17	-30235.809	5.2173174	-240166.79
CsF										
0	0	0	3.7449879	0.0030101	-4.59E-06	3.22E-09	-8.38E-13	-44090.696	7.1948735	-356483.91
1	0	0	4.4373309	1.27E-04	-2.05E-08	2.98E-12	-1.48E-16	-44227.995	3.8735562	-356483.91
CsO										
0	0	0	3.9857419	0.0021279	-3.22E-06	2.28E-09	-5.97E-13	6289.894	7.516023	62763.052
1	0	0	4.4660282	1.16E-04	-6.00E-09	1.32E-13	5.76E-17	6195.0309	5.2145491	62763.052
CsOH										
0	9386.96079	-500.93543	8.301352	-0.0032356	2.61E-06	-4.95E-10	-1.04E-13	-30257.224	-17.421948	-256000
1	896717.113	-2323.9786	7.9596449	1.10E-04	-6.47E-08	1.05E-11	-5.82E-16	-17362.582	-18.642396	-256000
CsOH+										
0	0	0	4.8487158	0.0068908	-1.18E-05	9.43E-09	-2.72E-12	51678.167	3.0848489	443519.62
1	0	0	5.7292563	0.0011571	-3.10E-07	3.71E-11	-1.55E-15	51626.483	-0.5764818	443519.62
Cs2										
0	0	0	4.7458823	-0.0026386	1.14E-05	-1.60E-08	6.56E-12	11544.486	7.6067932	107377.13
1	0	0	6.8664518	-0.0039901	1.32E-06	-1.63E-10	6.88E-15	10805.429	-4.2974942	107377.13
Cs2CL2										
0	0	0	9.2952642	0.0028506	-4.56E-06	3.26E-09	-8.61E-13	-82222.862	-7.518353	-659831.36
1	0	0	9.9424375	6.27E-05	-2.63E-08	4.89E-12	-3.36E-16	-82345.855	-10.59806	-659831.36
Cs2F2										
0	0	0	8.4425561	0.0064921	-1.08E-05	8.18E-09	-2.32E-12	-109781.65	-7.2482445	-890123.06
1	0	0	9.8793725	1.27E-04	-5.09E-08	8.97E-12	-5.81E-16	-110050.57	-14.054821	-890123.06
Cs2O										
0	0	0	5.7553639	0.0049116	-7.71E-06	5.42E-09	-1.41E-12	-12946.829	4.300155	-92046.757
1	0	0	6.8979467	1.02E-04	-3.81E-08	6.15E-12	-3.58E-16	-13169.989	-1.1659165	-92046.757
Cs2O2H2										
0	-10859.81041	-688.30684	16.435434	-0.0040392	2.33E-06	8.44E-10	-6.86E-13	-79394.762	-49.061968	-653000
1	1802857.941	-4656.3548	16.935666	2.12E-04	-1.27E-07	2.07E-11	-1.15E-15	-51908.137	-58.497192	-653000
Cs2SO4										
0	0	0	4.2965385	0.0448543	-6.10E-05	4.05E-08	-1.07E-11	-137825.59	13.409637	-1122581.4

1	0	0	15.419045	0.0040528	-1.79E-06	3.50E-10	-2.52E-14	-140367.75	-41.492185	-1122581.4
Cu										
0	77.1313315	-1.1692362	2.5069878	-2.12E-05	3.44E-08	-2.86E-11	9.56E-15	39839.812	5.7308132	337400
1	2308090.411	-8503.261	14.678591	-0.0084671	2.89E-06	-4.27E-10	2.30E-14	92075.356	-78.547016	337400
2	-6.49E+08	424032.34	-102.89658	0.0129726	-7.77E-07	2.22E-11	-2.44E-16	-3305304.6	919.86229	337400
Cu+										
0	4.17E-04	-5.72E-06	2.5	-9.36E-11	1.49E-13	-1.20E-16	3.85E-20	130240.06	5.07594	1089079.7
1	-2181443.045	7217.8582	-6.9411547	0.0062082	-2.14E-06	3.57E-10	-2.08E-14	85164.567	71.168006	1089079.7
2	2.99E+09	-1831416.2	429.49271	-0.0480193	2.84E-06	-8.45E-11	1.01E-15	1.47E+07	-3729.9181	1089079.7
Cu-										
0	0	0	2.5	0	0	0	0	24838.65	5.075966	212718.63
1	0	0	2.5	0	0	0	0	24838.65	5.075966	212718.63
2	0	0	2.5	0	0	0	0	24838.65	5.075966	212718.63
CuCL										
0	0	0	3.34916	0.0051028	-9.13E-06	7.60E-09	-2.40E-12	9796.7562	8.269473	91088.442
1	0	0	4.3902988	1.83E-04	-5.71E-08	1.13E-11	-8.20E-16	9609.7266	3.3921651	91088.442
CuF										
0	0	0	2.7654505	0.0068512	-1.13E-05	8.91E-09	-2.69E-12	-2554.8565	9.8727741	-12552.131
1	0	0	4.1227399	6.32E-04	-3.35E-07	8.08E-11	-5.78E-15	-2800.5953	3.4856457	-12552.131
CuF2										
0	0	0	3.1107696	0.0143258	-2.28E-05	1.73E-08	-5.07E-12	-33500.453	10.99957	-266945.9
1	0	0	6.8184236	-1.65E-04	2.03E-07	-2.55E-11	1.21E-16	-34322.744	-7.1286292	-266945.9
CuO										
0	0	0	3.709352	0.0031965	-5.30E-06	4.22E-09	-1.29E-12	35627.47	6.3314008	306276.72
1	0	0	4.2723625	4.47E-04	-2.40E-07	6.04E-11	-4.25E-15	35535.349	3.7270189	306276.72
Cu2										
0	0	0	3.9244358	0.0027275	-4.92E-06	4.18E-09	-1.34E-12	57119.187	6.0838083	485356.65
1	0	0	4.4239734	2.02E-04	-6.45E-08	1.41E-11	-7.60E-16	57038.131	3.7853558	485356.65
Cu3CL3										
0	0	0	11.4429	0.0206908	-3.83E-05	3.23E-08	-1.03E-11	-35151.61	-18.268787	-258575.3
1	0	0	15.626127	4.34E-04	-1.95E-07	3.85E-11	-2.79E-15	-35881.853	-37.752335	-258575.3
D										
0	0	0	2.5	0	0	0	0	25921.287	0.5917143	221720.23
1	60.5001921	-0.1810766	2.5002108	-1.22E-07	3.72E-11	-5.66E-15	3.39E-19	25922.438	0.5902125	221720.23
2	2.17E+08	-130930.99	33.925951	-0.003806	2.43E-07	-7.68E-12	9.62E-17	1065922	-272.62016	221720.23
D+										
0	0	0	2.5	0	0	0	0	184512	-0.1018415	1540324.3
1	0	0	2.5	0	0	0	0	184512	-0.1018415	1540324.3
2	0	0	2.5	0	0	0	0	184512	-0.1018415	1540324.3
D-										
0	0	0	2.5	0	0	0	0	16423.734	-0.1010243	142752.73
1	0	0	2.5	0	0	0	0	16423.734	-0.1010243	142752.73
2	0	0	2.5	0	0	0	0	16423.734	-0.1010243	142752.73
DBr										
0	-19450.7637	205.81448	3.0238123	-0.0014314	6.79E-06	-6.53E-09	2.08E-12	-6578.3038	8.1247459	-37036.447
1	665241.758	-2593.7019	6.8855111	-0.0011031	2.89E-07	-3.15E-11	1.01E-15	10375.577	-19.734336	-37036.447
DCL										
0	10464.209	-231.38133	5.4206932	-0.007508	1.40E-05	-1.07E-08	3.01E-12	-11284.034	-6.7118538	-93547.003
1	411728.335	-1764.5349	5.6688768	-3.48E-04	5.88E-08	3.76E-13	-5.16E-16	-1541.2601	-12.756604	-93547.003
DF										
0	57213.1092	-731.16656	7.2208397	-0.0094239	1.21E-05	-6.94E-09	1.54E-12	-30692.263	-19.327431	-276227
1	800115.502	-2438.3824	5.6206603	-2.02E-04	1.71E-08	2.70E-12	-2.89E-16	-18574.428	-14.730014	-276227
2	5.97E+07	-83312.607	34.560424	-0.0046509	3.67E-07	-1.41E-11	2.11E-16	580763.43	-257.70077	-276227
DOCL										
0	0	0	2.4790418	0.0108459	-1.52E-05	1.14E-08	-3.42E-12	-10518.092	12.126711	-78243.308
1	0	0	4.4350761	0.0025322	-1.03E-06	1.90E-10	-1.27E-14	-10919.402	2.7271597	-78243.308
DO2										
0	-21114.79735	602.33718	-1.2948777	0.0181295	-2.16E-05	1.39E-08	-3.70E-12	-2976.9439	32.728345	6487.344
1	-1267224.927	2799.947	2.3251746	0.0027263	-6.31E-07	6.73E-11	-2.77E-15	-19594.117	17.899228	6487.344
DO2-										
0	104870.5051	-890.62368	5.6665536	0.0019046	-1.22E-06	6.58E-10	-2.15E-13	-8942.3773	-7.7972192	-104795.51
1	552766.192	-2796.8958	8.7722067	-6.29E-04	1.27E-07	-1.36E-11	6.01E-16	2512.0668	-28.900204	-104795.51
D2										
0	21257.8989	-299.69451	5.1303145	-0.004173	5.01E-06	-2.13E-09	2.39E-13	394.49819	-11.64191	0
1	821515.641	-2365.6198	5.3429711	6.93E-05	-8.52E-08	2.46E-11	-1.96E-15	14342.124	-17.125979	0
2	4.90E+08	-311279.62	79.45732	-0.0084255	4.79E-07	-1.39E-11	1.64E-16	2460031	-663.681	0
D2+										
0	0	0	3.807514	-0.0031106	1.02E-05	-9.84E-09	3.27E-12	179170.96	-2.2866283	1498605.7
1	0	0	3.58918	8.92E-04	-2.43E-07	5.76E-11	-6.74E-15	179037.52	-2.0581789	1498605.7
D2-										
0	0	0	3.21448	7.84E-04	3.59E-06	-5.24E-09	2.09E-12	27293.009	0.3681558	235371.94
1	0	0	3.7531042	9.80E-04	-3.64E-07	7.07E-11	-5.07E-15	27064.708	-2.8195517	235371.94
D2O										
0	6958.27847	-12.808894	3.5958789	0.0015021	3.59E-07	5.34E-10	-5.18E-13	-31019.446	2.8955566	-249210
1	1544193.253	-5474.2389	10.175424	-9.62E-04	2.04E-07	-2.05E-11	8.51E-16	2983.249	-44.650116	-249210
D2O2										
0	29577.11324	-68.930376	2.0439055	0.0157028	-1.94E-05	1.38E-08	-4.10E-12	-18025.027	13.471565	-144300
1	1147867.936	-5225.7609	13.110887	-0.0011798	2.73E-07	-2.96E-11	1.31E-15	12195.805	-56.905382	-144300
D2S										
0	0	0	3.8070824	3.76E-04	5.75E-06	-5.35E-09	1.41E-12	-4066.1219	3.8792875	-23890.981
1	0	0	3.6662901	0.0034992	-1.42E-06	2.67E-10	-1.87E-14	-4214.7308	3.7996997	-23890.981
F										

0	1137.409088	-145.33928	4.0774036	-0.0043034	5.73E-06	-3.82E-09	1.02E-12	9311.1101	-3.5589827	79380
1	14735.06226	81.499274	2.4443718	2.12E-05	-4.55E-09	5.11E-13	-2.33E-17	8388.3747	5.4787106	79380
2	-2.93E+07	17756.749	-1.8144633	5.35E-04	-3.51E-08	1.10E-12	-1.06E-17	-131964.27	42.488146	79380
F+										
0	-38716.8019	321.88157	2.2009205	-2.46E-04	7.86E-07	-6.44E-10	1.84E-13	209883.09	7.8169992	1766816.3
1	16496.35664	133.73515	2.3325229	1.22E-04	-4.80E-08	9.03E-12	-5.47E-16	211074.53	6.6258171	1766816.3
2	7599619.33	-1391.1066	1.7148715	2.43E-04	-1.89E-08	6.42E-13	-8.26E-18	226912.6	11.028489	1766816.3
F-										
0	0	0	2.5	0	0	0	0	-31425.724	3.2648827	-255092.07
1	0	0	2.5	0	0	0	0	-31425.724	3.2648827	-255092.07
2	0	0	2.5	0	0	0	0	-31425.724	3.2648827	-255092.07
FCN										
0	39844.5412	-698.86554	7.0588397	-0.0014049	3.96E-06	-3.05E-09	7.92E-13	6172.6276	-15.05643	34327.854
1	398187.355	-2302.9711	9.0270814	-5.23E-04	1.19E-07	-1.28E-11	5.73E-16	15884.495	-29.849718	34327.854
FO										
0	-39121.8244	796.70369	-1.6347778	0.0160181	-2.10E-05	1.38E-08	-3.66E-12	8375.5252	33.833257	109012.1
1	-1597940.503	4377.3764	-0.4897508	0.0026823	-6.90E-07	7.25E-11	-2.73E-15	-16442.482	35.599236	109012.1
FO2,FOO										
0	5819.12126	-234.68972	5.4370037	0.002167	3.65E-07	-2.07E-09	9.43E-13	2694.6452	-1.1664145	25400
1	-1213177.293	2493.4361	4.4650388	9.42E-04	-6.43E-08	-1.09E-11	1.22E-15	-15968.252	8.6554175	25400
FO2,OFO										
0	-77341.064	1663.8002	-9.6128152	0.0498916	-6.95E-05	4.71E-08	-1.26E-11	36970.927	77.95943	378600
1	-621186.734	936.94746	6.4015588	2.14E-04	-4.34E-08	4.67E-12	-2.06E-16	36383.573	-6.1502643	378600
F2										
0	10181.76308	22.742412	1.971353	0.0081516	-1.15E-05	7.96E-09	-2.17E-12	-958.6943	11.306003	0
1	-2941167.79	9456.5977	-7.7386162	0.0076447	-2.24E-06	2.92E-10	-1.43E-14	-60710.056	84.238351	0
F2O										
0	30829.19995	-229.95063	2.6038058	0.0158611	-2.35E-05	1.68E-08	-4.70E-12	3055.1853	10.50933	24500
1	-188537.4518	-210.07297	7.1512392	1.33E-04	1.80E-08	-1.42E-12	6.49E-17	1449.13	-12.578583	24500
F2O2										
0	56122.7046	-998.59522	8.9806494	0.0064219	-9.89E-06	6.86E-09	-1.84E-12	5298.7126	-22.392922	19200
1	-219056.3532	-391.09208	10.291071	-1.16E-04	2.57E-08	-2.95E-12	1.37E-16	827.80209	-27.567526	19200
FS2F,fluorodisu										
0	114446.228	-1853.2476	13.940985	-0.0040437	1.37E-06	6.71E-10	-4.62E-13	-33510.683	-48.492124	-336435
1	-207709.7921	-109.45398	10.081369	-3.24E-05	7.13E-09	-8.13E-13	3.76E-17	-43494.461	-23.469131	-336435
Fe										
0	67908.2266	-1197.2184	9.8433933	-0.0165232	1.92E-05	-1.15E-08	2.83E-12	54669.959	-33.839463	415471
1	-1954923.682	6737.1611	-5.486411	0.0043788	-1.12E-06	1.54E-10	-8.02E-15	7137.3701	65.049799	415471
2	1.22E+09	-582856.39	97.896345	-0.0053707	3.19E-08	6.27E-12	-1.48E-16	4847648.3	-869.72898	415471
Fe+										
0	-56912.3162	184.71344	4.1969721	-0.0059783	1.05E-05	-8.06E-09	2.26E-12	140120.66	-0.3602543	1184217.8
1	-817645.009	1925.3594	1.7173872	3.39E-04	-9.81E-08	2.23E-11	-1.48E-15	128635.25	15.002563	1184217.8
2	1.07E+08	-28839.24	-2.8217525	0.0027128	-3.11E-07	1.54E-11	-2.73E-16	414298.17	40.534973	1184217.8
Fe-										
0	134127.6767	-1775.4381	10.843669	-0.0149944	1.41E-05	-6.94E-09	1.41E-12	55194.725	-41.408865	393338.04
1	-123780.8631	824.92791	1.9129365	2.28E-04	-4.94E-08	5.59E-12	-2.57E-16	41562.516	12.653676	393338.04
2	-1008467.687	764.24024	2.3328803	1.89E-05	-1.17E-09	3.75E-14	-4.87E-19	41114.172	9.6809218	393338.04
FeC5O5										
0	0	0	6.606546	0.0750421	-1.22E-04	1.01E-07	-3.23E-11	-91951.438	-2.5760445	-727858.87
1	0	0	21.164021	0.0103331	-4.33E-06	8.20E-10	-5.78E-14	-94888.934	-72.07369	-727858.87
FeCL										
0	0	0	3.7885826	0.0043678	-6.69E-06	4.17E-09	-8.47E-13	28920.097	8.3533347	251035.97
1	0	0	4.6940669	1.16E-04	-2.08E-08	-1.76E-12	5.23E-16	28790.344	4.1935222	251035.97
FeCL2										
0	0	0	5.4557505	0.0079633	-1.26E-05	9.00E-09	-2.32E-12	-18844.297	3.0228185	-140999.99
1	0	0	6.9492601	5.34E-04	7.02E-08	-6.15E-11	6.79E-15	-19045.832	-3.7595381	-140999.99
FeCL3										
0	0	0	7.5614873	0.0097338	-1.55E-05	1.12E-08	-3.00E-12	-33013.624	-3.9858505	-253119.99
1	0	0	9.7771106	2.44E-04	-1.03E-07	1.92E-11	-1.32E-15	-33439.57	-14.549165	-253119.99
FeO										
0	0	0	2.8245256	0.0043049	-4.11E-06	1.32E-09	7.13E-14	29194.035	11.891134	251047.08
1	0	0	4.2049817	2.68E-04	-8.94E-08	3.19E-11	-3.39E-15	28829.17	4.8303898	251047.08
Fe(OH)2										
0	0	0	-1.6766773	0.0616931	-1.21E-04	1.10E-07	-3.73E-11	-41128.971	29.677138	-330536
1	0	0	8.9626201	0.0042014	-1.61E-06	2.68E-10	-1.63E-14	-42799.436	-18.69127	-330536
Fe2CL4										
0	0	0	12.738242	0.0132356	-2.16E-05	1.60E-08	-4.35E-12	-56106.579	-19.824773	-431373.78
1	0	0	15.3575	6.42E-04	2.08E-08	-5.16E-11	6.07E-15	-56510.037	-31.896611	-431373.78
Fe2CL6										
0	0	0	14.221181	0.0435486	-9.60E-05	9.37E-08	-3.36E-11	-84199.627	-25.924488	-654377.6
1	0	0	21.564503	4.62E-04	-1.85E-07	3.20E-11	-2.01E-15	-85243.238	-58.653837	-654377.6
GaBr										
0	-2185.275415	-76.72233	4.7708057	-4.50E-04	5.58E-07	-3.07E-10	7.04E-14	-3138.0048	2.9481443	-17967.88
1	335980.503	-840.68367	5.1450847	-3.27E-05	-7.67E-08	3.64E-11	-3.36E-15	2035.1794	-0.4277894	-17967.88
GaBr2										
0	7081.68162	-370.57661	8.4184254	-0.0030019	3.60E-06	-2.28E-09	5.91E-13	-18211.167	-9.5125721	-149180.95
1	-330229.436	476.67227	7.1047254	-5.52E-04	3.16E-07	-5.51E-11	3.17E-15	-23656.836	-1.1627149	-149180.95
GaBr3										
0	6363.80734	-514.20405	11.960651	-0.0041346	4.93E-06	-3.11E-09	8.04E-13	-35704.155	-25.568961	-292962.66
1	-51030.6375	-9.3952097	10.007688	-3.30E-06	7.68E-10	-9.18E-14	4.39E-18	-38334.022	-14.103159	-292962.66
GaCL										
0	6417.143	-225.79491	5.3116737	-0.0015623	1.84E-06	-1.10E-09	2.73E-13	-8593.8923	-1.695916	-69621.44

1	-486484.224	1452.8702	2.719543	0.0011443	-3.43E-07	5.47E-11	-3.02E-15	-18950.84	15.709257	-69621.44
GaCL2										
0	22254.81851	-604.62184	9.2203889	-0.0045544	5.32E-06	-3.31E-09	8.46E-13	-25645.504	-16.854099	-220978.91
1	-344540.53	471.44372	7.1087755	-5.54E-04	3.16E-07	-5.52E-11	3.18E-15	-32309.362	-3.7448471	-220978.91
GaCL3										
0	47849.484	-1162.6781	14.089542	-0.0081061	9.22E-06	-5.60E-09	1.40E-12	-49159.097	-42.821802	-432624.75
1	-94669.1731	-25.614683	10.0201	-8.35E-06	1.90E-09	-2.23E-13	1.05E-17	-55182.014	-18.649592	-432624.75
GaF										
0	36703.9801	-533.65722	5.7592919	-0.0015061	9.51E-07	-1.83E-10	-3.14E-14	-26470.757	-6.5893219	-232608.49
1	-298339.2279	722.51579	3.6395574	5.55E-04	-1.46E-07	2.18E-11	-1.03E-15	-34085.287	7.55396	-232608.49
GaF2										
0	68425.3953	-889.76177	7.7074555	0.0020722	-5.29E-06	4.56E-09	-1.41E-12	-59198.562	-13.411421	-516712.44
1	410025.136	-1723.2595	8.9513292	-0.0010592	2.75E-07	-2.91E-11	1.08E-15	-53765.716	-21.138355	-516712.44
GaF3										
0	95932.667	-1355.5075	10.977602	0.0034616	-8.47E-06	7.22E-09	-2.21E-12	-106147.91	-32.126519	-921476.98
1	-209696.176	-143.12113	10.105684	-4.18E-05	9.16E-09	-1.04E-12	4.80E-17	-113667.81	-23.925393	-921476.98
GaH										
0	-43918.762	625.44571	0.3276863	0.0064966	-3.80E-06	2.85E-10	3.63E-13	21712.601	22.240322	214323.4
1	3257993.99	-11090.995	18.011268	-0.0081677	2.60E-06	-3.81E-10	2.03E-14	93697.782	-98.209002	214323.4
GaI										
0	-3661.85503	-32.069242	4.5999619	-8.90E-05	1.16E-07	-1.81E-11	-7.58E-15	4198.6494	4.9289647	44871.122
1	1498356.654	-4551.9672	9.8030054	-0.0029437	8.66E-07	-1.11E-10	5.01E-15	32918.119	-32.273598	44871.122
GaI2										
0	-983.13959	-215.26213	7.8443188	-0.0018198	2.21E-06	-1.42E-09	3.71E-13	-4534.0902	-4.2505168	-28954.965
1	-320287.975	479.65023	7.102334	-5.51E-04	3.16E-07	-5.51E-11	3.17E-15	-9180.9196	0.7275205	-28954.965
GaI3										
0	-5663.47265	-242.59371	10.954511	-0.0020592	2.50E-06	-1.60E-09	4.17E-13	-15767.228	-16.461299	-115877.24
1	-31640.4013	-4.2086628	10.00352	-1.53E-06	3.61E-10	-4.35E-14	2.10E-18	-17000.585	-10.902916	-115877.24
GaO										
0	73255.4391	-980.42695	7.8441228	-0.0071711	7.87E-06	-2.40E-09	-2.59E-13	21405.817	-17.99743	146823.61
1	2937313.804	-11183.141	18.593668	-0.0068548	1.67E-06	-1.89E-10	7.97E-15	85302.481	-99.040405	146823.61
GaOH										
0	69631.0187	-1247.8287	10.220016	-0.0059225	4.64E-06	-1.22E-09	-2.95E-14	-12753.978	-32.17063	-143630.5
1	842905.101	-2372.3246	8.0090711	8.78E-05	-5.94E-08	9.84E-12	-5.53E-16	-3751.7883	-21.710537	-143630.5
Ga2Br2										
0	-11171.83241	-74.714716	10.302461	-6.66E-04	8.20E-07	-5.30E-10	1.39E-13	-19132.979	-13.171103	-136963.69
1	-18853.73131	-1.2636218	10.00108	-4.77E-07	1.14E-10	-1.38E-14	6.69E-19	-19510.538	-11.416676	-136963.69
Ga2Br4										
0	-13155.45939	-413.6553	17.628492	-0.0035147	4.27E-06	-2.73E-09	7.12E-13	-52831.018	-44.275207	-415820.03
1	-57421.6721	-7.1601374	16.005989	-2.61E-06	6.15E-10	-7.41E-14	3.57E-18	-54933.898	-34.792717	-415820.03
Ga2Br6										
0	-6725.11689	-806.75266	25.116714	-0.0066365	7.98E-06	-5.06E-09	1.31E-12	-83706.352	-75.852787	-673688.73
1	-95261.73	-14.446819	22.011925	-5.15E-06	1.20E-09	-1.44E-13	6.93E-18	-87822.233	-57.658951	-673688.73
Ga2CL2										
0	-9246.1337	-259.21599	11.028471	-0.002232	2.72E-06	-1.74E-09	4.56E-13	-28340.598	-20.677737	-220972.69
1	-36689.542	-4.4345807	10.003731	-1.63E-06	3.85E-10	-4.65E-14	2.24E-18	-29656.331	-14.695362	-220972.69
Ga2CL4										
0	16373.43702	-1140.6374	20.301398	-0.0089977	1.07E-05	-6.70E-09	1.73E-12	-71623.85	-66.663625	-602326.83
1	-112711.0409	-21.385175	16.017381	-7.42E-06	1.72E-09	-2.05E-13	9.80E-18	-77468.534	-41.472815	-602326.83
Ga2CL6										
0	60894.6984	-2104.4563	29.596539	-0.0153781	1.78E-05	-1.10E-08	2.78E-12	-111840.05	-112.19459	-962463.53
1	-189844.5426	-44.136552	22.03505	-1.47E-05	3.37E-09	-3.98E-13	1.88E-17	-122697	-67.453337	-962463.53
Ga2F2										
0	29781.3065	-1013.9755	13.749331	-0.0077281	9.06E-06	-5.64E-09	1.44E-12	-70860.834	-41.09834	-606231.34
1	-87732.3493	-19.837759	10.01594	-6.74E-06	1.56E-09	-1.85E-13	8.78E-18	-76073.686	-19.083255	-606231.34
Ga2F4										
0	142207.9998	-2798.8299	23.959042	-0.012939	1.22E-05	-6.25E-09	1.33E-12	-149601.37	-97.341536	-1325003
1	-270436.609	-104.99572	16.07904	-3.18E-05	7.05E-09	-8.10E-13	3.76E-17	-164416.96	-48.965917	-1325003
Ga2F6										
0	240904.5572	-4142.3798	31.957737	-0.0129791	8.96E-06	-2.73E-09	1.55E-13	-227278.52	-139.84037	-2017623.8
1	-436866.48	-212.82084	22.158864	-6.35E-05	1.40E-08	-1.60E-12	7.41E-17	-249429.87	-77.876358	-2017623.8
Ga2I2										
0	-8960.25267	-31.720572	10.129305	-2.86E-04	3.54E-07	-2.29E-10	6.04E-14	-1233.1741	-9.8019684	13520.947
1	-12190.56501	-0.5287554	10.000454	-2.01E-07	4.80E-11	-5.83E-15	2.83E-19	-1393.2586	-9.0526149	13520.947
Ga2I4										
0	-17694.95991	-135.48715	16.546253	-0.001199	1.47E-06	-9.50E-10	2.50E-13	-23334.058	-33.257129	-159267.99
1	-31712.9976	-2.2870688	16.001948	-8.59E-07	2.04E-10	-2.48E-14	1.20E-18	-24019.405	-30.086725	-159267.99
Ga2I6										
0	-21108.91458	-369.54042	23.468118	-0.0031892	3.89E-06	-2.49E-09	6.53E-13	-43011.881	-60.148115	-317294.62
1	-60156.9815	-6.3292092	22.00533	-2.33E-06	5.51E-10	-6.66E-14	3.21E-18	-44886.994	-51.610088	-317294.62
Ga2O										
0	56971.9718	-807.4086	7.7330615	0.0014785	-4.10E-06	3.58E-09	-1.11E-12	-9512.2168	-12.561493	-99457.457
1	-119387.4986	-87.193416	7.0646782	-2.57E-05	5.65E-09	-6.45E-13	2.98E-17	-13936.948	-6.9428013	-99457.457
Ge										
0	-20592.15242	-143.20221	4.5060023	0.0015472	-8.52E-06	8.24E-09	-2.57E-12	43630.709	-6.2252685	367800
1	-856541.384	3917.9587	-1.8098882	0.0022765	-5.37E-07	5.98E-11	-2.54E-15	19565.188	38.413468	367800
2	2.42E+07	-25436.052	14.560875	-0.0025926	2.66E-07	-1.12E-11	1.62E-16	229581.25	-89.535859	367800
Ge+										
0	-345366.643	4008.4497	-15.223957	0.0362603	-3.35E-05	1.43E-08	-2.24E-12	115705.8	109.0152	1134984.4
1	-2244860.57	5165.5311	-0.3867517	8.53E-04	-1.39E-07	1.16E-11	-3.78E-16	100682.4	29.657834	1134984.4
2	5.77E+07	-30786.062	8.7062918	-4.94E-04	-2.69E-11	1.85E-12	-5.08E-17	385778.54	-48.425991	1134984.4
Ge-										

0	2989.142308	86.574172	2.1918685	5.90E-04	-6.38E-07	3.66E-10	-8.69E-14	28356.952	9.417004	245402.54
1	13520.40246	-0.5048519	2.5001402	-3.65E-09	-6.72E-12	1.38E-15	-8.48E-20	28817.398	7.5773343	245402.54
2	10798.77187	1.1499692	2.499738	3.05E-08	-1.93E-12	6.31E-17	-8.33E-22	28804.297	7.5808477	245402.54
GeBr										
0	-56715.5794	916.86036	-2.2250657	0.0217236	-3.04E-05	2.01E-08	-5.21E-12	11045.088	41.08177	137440.77
1	-741799.553	2259.5064	2.6694697	9.31E-04	-2.47E-07	3.63E-11	-1.82E-15	525.95955	19.395225	137440.77
GeBr2										
0	-1649.73847	-229.624	7.900161	-0.0019368	2.35E-06	-1.50E-09	3.90E-13	-8316.6396	-6.9184102	-60962.897
1	-26255.592	-4.3225236	7.0037088	-1.66E-06	4.02E-10	-4.99E-14	2.47E-18	-9482.8878	-1.676536	-60962.897
GeBr3										
0	2725.568677	-518.62133	11.999578	-0.004251	5.10E-06	-3.23E-09	8.39E-13	-14779.883	-25.345701	-119031.31
1	-54339.267	-9.280328	10.00765	-3.30E-06	7.71E-10	-9.24E-14	4.43E-18	-17426.971	-13.669607	-119031.31
GeBr4										
0	5431.94039	-677.77488	15.600153	-0.0055078	6.59E-06	-4.17E-09	1.08E-12	-35576.064	-42.091344	-291000
1	-69777.5791	-11.798731	13.00954	-4.02E-06	9.20E-10	-1.08E-13	5.04E-18	-39041.482	-26.894475	-291000
GeCL										
0	13126.2484	-57.927195	2.1849139	0.0131389	-2.28E-05	1.73E-08	-4.94E-12	7610.3957	13.954768	69027.753
1	-488269.322	1657.7815	3.0958198	7.28E-04	-1.84E-07	2.58E-11	-1.21E-15	-3657.9946	14.750586	69027.753
GeCL2										
0	18384.8083	-582.71177	9.161352	-0.0044646	5.24E-06	-3.27E-09	8.37E-13	-19758.027	-17.343247	-171000
1	-48860.5225	-11.369524	7.0091747	-3.90E-06	9.02E-10	-1.07E-13	5.12E-18	-22751.849	-4.6577657	-171000
GeCL3										
0	19355.2244	-834.15631	13.126789	-0.0065108	7.70E-06	-4.82E-09	1.24E-12	-30972.409	-35.524396	-266950.59
1	-75946.5007	-15.229994	10.012179	-5.11E-06	1.17E-09	-1.37E-13	6.44E-18	-35254.929	-17.193076	-266950.59
GeCL4										
0	65028.7041	-1652.4828	18.81327	-0.0115243	1.31E-05	-7.96E-09	2.00E-12	-55700.524	-67.5446	-500000
1	-137626.121	-36.037695	13.028167	-1.16E-05	2.64E-09	-3.07E-13	1.44E-17	-64262.818	-33.181801	-500000
GeF										
0	53103.6898	-483.28279	3.2449765	0.0118066	-2.23E-05	1.76E-08	-5.17E-12	-6885.9191	5.6650873	-70591.091
1	-432401.774	1386.3619	3.3599274	5.75E-04	-1.38E-07	1.83E-11	-7.76E-16	-18808.579	11.219508	-70591.091
GeF2										
0	75434.361	-1108.5059	9.0791789	-0.0014464	-6.56E-07	1.47E-09	-5.81E-13	-65106.62	-22.006532	-574000
1	-127533.758	-71.627406	7.0530116	-2.10E-05	4.61E-09	-5.25E-13	2.42E-17	-71126.372	-8.4843057	-574000
GeF3										
0	111406.378	-1776.8248	13.521198	-0.0029823	-3.81E-08	1.62E-09	-7.20E-13	-90383.028	-45.685358	-806332.83
1	-206897.093	-111.20603	10.082547	-3.28E-05	7.22E-09	-8.24E-13	3.80E-17	-99996.327	-23.036483	-806332.83
GeF4										
0	111983.341	-1636.884	12.313873	0.0102539	-1.89E-05	1.48E-08	-4.32E-12	-137426.4	-41.043203	-1190150
1	-325332.222	-253.77134	13.18789	-7.46E-05	1.64E-08	-1.87E-12	8.61E-17	-146618.04	-41.222421	-1190150
GeI										
0	-74333.0469	1033.6496	-1.516945	0.0155383	-1.68E-05	8.37E-09	-1.55E-12	19130.136	39.593453	210975.08
1	-949987.339	2470.8784	2.8130924	8.43E-04	-2.32E-07	3.81E-11	-2.06E-15	7588.1188	19.473581	210975.08
GeO										
0	-5705.12181	264.06419	0.6993936	0.0109159	-1.47E-05	9.89E-09	-2.64E-12	-6638.8491	21.11885	-37693.701
1	-2160611.93	6045.063	-2.4724762	0.0039171	-1.08E-06	1.35E-10	-4.60E-15	-44699.411	50.492153	-37693.701
GeO2										
0	-3824.17383	156.34516	1.6941983	0.0175621	-2.42E-05	1.63E-08	-4.37E-12	-14775.349	15.568835	-106172
1	-172734.7526	-296.11544	7.7207263	-8.82E-05	1.95E-08	-2.24E-12	1.04E-16	-13879.833	-16.698887	-106172
GeS										
0	34990.4951	-544.11954	6.0405248	-0.0024498	2.31E-06	-1.16E-09	2.42E-13	12636.817	-7.0688255	92537.497
1	-3566535.44	10997.382	-8.9710426	0.0082418	-2.60E-06	3.96E-10	-2.11E-14	-59723.551	97.680111	92537.497
GeS2										
0	55436.836	-1024.8267	10.575946	-0.0052879	5.30E-06	-2.87E-09	6.52E-13	17355.797	-29.917502	118817.83
1	-89709.8036	-33.64377	7.5254337	-1.03E-05	2.28E-09	-2.63E-13	1.22E-17	11952.321	-11.352013	118817.83
Ge2										
0	213763.063	-3044.3326	18.681832	-0.0254725	2.20E-05	-8.42E-09	9.66E-13	70155.43	-77.90904	471505.89
1	1395098.81	-3279.462	7.9230806	-0.0015282	4.32E-07	-4.88E-11	1.98E-15	77026.895	-18.959591	471505.89
H										
0	0	0	2.5	0	0	0	0	25473.708	-0.4466829	217998.83
1	60.7877425	-0.1819354	2.5002118	-1.23E-07	3.73E-11	-5.69E-15	3.41E-19	25474.864	-0.4481918	217998.83
2	2.17E+08	-131203.54	33.991742	-0.003814	2.43E-07	-7.69E-12	9.64E-17	1067638.1	-274.23011	217998.83
H+										
0	0	0	2.5	0	0	0	0	184021.49	-1.1406466	1536245.9
1	0	0	2.5	0	0	0	0	184021.49	-1.1406466	1536245.9
2	0	0	2.5	0	0	0	0	184021.49	-1.1406466	1536245.9
H-										
0	0	0	2.5	0	0	0	0	15976.155	-1.1390139	139031.33
1	0	0	2.5	0	0	0	0	15976.155	-1.1390139	139031.33
2	0	0	2.5	0	0	0	0	15976.155	-1.1390139	139031.33
HALO										
0	26686.08286	-466.3133	5.3837604	0.0029025	-2.24E-07	-1.52E-09	6.95E-13	1235.8744	-6.5086103	1821.114
1	78457.1898	-1515.5845	8.5727331	-4.14E-04	8.93E-08	-1.01E-11	4.61E-16	6662.9525	-26.729172	1821.114
HALO2										
0	3544.59891	115.98191	0.8637971	0.0246088	-3.42E-05	2.37E-08	-6.47E-12	-44495.061	20.123171	-355473.55
1	698570.544	-2864.935	10.867215	-5.37E-05	-2.84E-08	6.29E-12	-3.89E-16	-27643.925	-37.758863	-355473.55
HBO										
0	63609.7503	-800.15576	6.2188161	-7.80E-04	3.14E-06	-2.03E-09	3.74E-13	-22402.829	-13.269524	-210621.21
1	886186.023	-3913.0681	9.8886448	-8.22E-04	1.62E-07	-1.70E-11	7.37E-16	-3161.852	-40.368127	-210621.21
HBO+										
0	0	0	2.2544283	0.0080302	-5.97E-06	2.43E-09	-4.31E-13	141850.69	10.812208	1187574.5
1	0	0	3.947508	0.0034315	-1.28E-06	2.22E-10	-1.48E-14	141359.98	1.998896	1187574.5
HBO-										

0	0	0	3.9707955	-0.00221	1.45E-05	-1.56E-08	5.40E-12	-30589.499	4.8249697	-244477.96
1	0	0	4.0869265	0.0029785	-1.24E-06	2.47E-10	-1.85E-14	-30930.026	2.7801425	-244477.96
HBO2										
0	6225.08747	75.661537	1.2534068	0.0174801	-1.98E-05	1.23E-08	-3.15E-12	-68785.888	17.677935	-560210.05
1	1049369.185	-4479.1455	11.977559	-4.74E-04	6.08E-08	-3.64E-12	6.16E-17	-42211.495	-49.113668	-560210.05
HBS										
0	0	0	1.5595903	0.0139668	-1.80E-05	1.23E-08	-3.41E-12	5089.0936	13.501899	50208.558
1	0	0	4.4412265	0.002998	-1.19E-06	2.12E-10	-1.35E-14	4440.2975	-0.6467832	50208.558
HBS+										
0	0	0	2.2511561	0.0120772	-1.53E-05	1.05E-08	-2.93E-12	134754.76	11.27077	1129498.9
1	0	0	4.7097542	0.0028187	-1.16E-06	2.18E-10	-1.51E-14	134191.39	-0.8374721	1129498.9
HBr										
0	25272.22498	-406.51103	6.0431166	-0.0077179	1.15E-05	-7.29E-09	1.75E-12	-3510.4146	-9.9031863	-36290
1	1170033.949	-3786.521	7.5031481	-0.001285	3.21E-07	-3.44E-11	1.13E-15	18564.133	-25.627129	-36290
HCN										
0	90982.9783	-1238.6597	8.7213223	-0.0065283	8.87E-06	-4.81E-09	9.32E-13	21219.79	-27.466867	135000
1	1236898.25	-4446.7618	9.7389116	-5.86E-04	1.07E-07	-1.01E-11	3.35E-16	42445.948	-40.058008	135000
HCO										
0	-11899.06845	215.16118	2.730184	0.0018066	4.98E-06	-5.81E-09	1.87E-12	2905.7191	11.367935	42397.85
1	691133.57	-3643.2178	9.5870849	-0.0011049	2.83E-07	-3.54E-11	1.74E-15	25356.227	-35.701987	42397.85
HCO+										
0	118316.517	-1604.6676	10.671712	-0.011689	1.61E-05	-9.98E-09	2.38E-12	106939.57	-38.203399	833000
1	1203649.25	-4460.9802	9.932598	-7.54E-04	1.35E-07	-1.30E-11	5.22E-16	126349.21	-41.066993	833000
2	-1518062.38	-552.66808	7.610716	-1.19E-05	7.05E-10	-2.20E-14	2.79E-19	98744.602	-23.054717	833000
HCCN										
0	2992.8514	-440.4484	6.9399393	0.0038466	-1.27E-06	-3.64E-10	2.75E-13	73708.701	-13.152507	610430.63
1	939576.184	-4091.1157	12.722392	-6.87E-04	1.23E-07	-1.19E-11	4.76E-16	95851.948	-52.487398	610430.63
HCL										
0	20625.88287	-309.33689	5.2754189	-0.0048289	6.20E-06	-3.04E-09	4.92E-13	-10677.823	-7.3093178	-92310
1	915774.951	-2770.5502	5.9735398	-3.63E-04	4.74E-08	2.81E-12	-6.66E-16	5674.9581	-16.428271	-92310
HD										
0	25191.20338	-276.1005	4.6444413	-0.0020824	1.42E-06	2.84E-10	-3.20E-13	391.36164	-9.3953961	323.302
1	845583	-1956.5785	4.4043739	5.75E-04	-2.13E-07	4.04E-11	-2.73E-15	12272.542	-10.847429	323.302
2	4.83E+08	-307714.49	78.648165	-0.008333	4.73E-07	-1.37E-11	1.61E-16	2431070.4	-656.94371	323.302
HD+										
0	0	0	3.8827136	-0.0030779	8.19E-06	-6.81E-09	1.99E-12	178945.63	-2.8033598	1496830.5
1	0	0	3.2909764	0.0011552	-3.44E-07	7.67E-11	-8.09E-15	178942.79	-0.4786072	1496830.5
HD-										
0	0	0	3.6428877	-0.0021291	8.93E-06	-9.35E-09	3.26E-12	27269.271	-2.2556266	235489.46
1	0	0	3.4939949	0.0012449	-4.73E-07	9.11E-11	-6.49E-15	27157.734	-2.2311046	235489.46
HDO										
0	-27377.95356	431.05039	1.5584799	0.005765	-4.86E-06	3.38E-09	-1.04E-12	-32732.265	14.877519	-245280.48
1	1711376.798	-5322.8723	9.1243515	-3.40E-04	4.15E-08	-4.78E-14	-1.47E-16	3245.2247	-37.746007	-245280.48
HDO2										
0	-32164.9965	749.23672	-1.9576941	0.0241281	-2.92E-05	1.93E-08	-5.23E-12	-21509.418	36.724167	-140231.74
1	1313170.99	-5175.6149	12.164891	-6.14E-04	1.23E-07	-1.08E-11	3.87E-16	13033.139	-50.85263	-140231.74
HDO2										
0	-32164.9965	749.23672	-1.9576941	0.0241281	-2.92E-05	1.93E-08	-5.23E-12	-21509.418	36.724167	-140231.74
1	1313170.99	-5175.6149	12.164891	-6.14E-04	1.23E-07	-1.08E-11	3.87E-16	13033.139	-50.85263	-140231.74
HF										
0	-3192.09897	59.868077	3.0551139	0.0016847	-3.29E-06	3.10E-09	-9.76E-13	-34184.432	3.2949041	-273300
1	725708.904	-1484.7977	3.8555275	7.14E-04	-2.11E-07	3.05E-11	-1.64E-15	-23554.567	-3.2038568	-273300
2	1.76E+08	-87899.981	18.865249	-6.85E-04	-1.40E-08	1.50E-12	-2.72E-17	685357.32	-139.32316	-273300
HI										
0	0	0	3.6963722	-0.0014225	3.01E-06	-1.27E-09	-3.51E-14	2107.3581	4.0881211	26359.556
1	0	0	2.9104008	0.0015688	-5.92E-07	1.05E-10	-7.04E-15	2250.8659	7.8644705	26359.556
HNC										
0	48704.0453	-989.11382	9.7219706	-0.0111354	1.67E-05	-1.11E-08	2.89E-12	26646.646	-31.047266	194378.12
1	1198765.94	-3918.8753	9.1179531	-3.42E-04	3.31E-08	-5.69E-13	-7.79E-17	46587.67	-34.685287	194378.12
HNCO										
0	75712.1962	-955.63856	6.7083219	0.0047746	-5.09E-06	3.81E-09	-1.20E-12	-10674.963	-13.576859	-118061.4
1	1257367.696	-5038.2397	12.496174	-6.98E-04	1.12E-07	-9.54E-12	3.35E-16	14636.983	-53.205799	-118061.4
HNO										
0	-68547.9088	955.16534	-0.6000762	0.0079951	-6.55E-07	-3.67E-09	1.78E-12	6435.3373	30.4817	102032.73
1	-5797632.99	19463.134	-21.538761	0.0179832	-4.98E-06	6.40E-10	-3.14E-14	-110470.95	181.95524	102032.73
HNO2										
0	8591.98506	120.3644	0.9412979	0.0194289	-2.25E-05	1.38E-08	-3.47E-12	-11063.372	20.739675	-78451.922
1	878790.413	-3990.455	11.873493	-4.88E-04	7.13E-08	-5.38E-12	1.58E-16	12463.432	-46.088746	-78451.922
HNO3										
0	9202.86901	109.37745	-0.4521042	0.0298491	-3.19E-05	1.72E-08	-3.78E-12	-17640.485	27.46645	-133912.87
1	-94978.0964	-2733.0245	14.49427	-7.82E-04	1.70E-07	-1.93E-11	8.87E-16	-4882.5178	-59.283929	-133912.87
HOCL										
0	-9892.42208	356.90444	0.144294	0.0161825	-2.18E-05	1.51E-08	-4.12E-12	-11773.703	24.793036	-75740.849
1	853238.909	-2849.4477	7.9498267	-1.06E-04	-1.47E-08	4.57E-12	-3.05E-16	7260.8681	-22.508344	-75740.849
HOF										
0	-36969.3793	780.90771	-2.0777243	0.020387	-2.59E-05	1.71E-08	-4.55E-12	-16317.235	36.450742	-96898.221
1	881185.028	-3119.9705	8.2236684	-2.30E-04	1.46E-08	1.10E-12	-1.40E-16	6300.2683	-25.9012	-96898.221
HO2										
0	-75988.8254	1329.3839	-4.6773882	0.0250831	-3.01E-05	1.90E-08	-4.83E-12	-5809.3664	51.936021	12552
1	-1810669.724	4963.192	-1.039499	0.0045601	-1.06E-06	1.14E-10	-4.76E-15	-31944.187	40.668509	12552
HO2-										
0	598.051765	453.21837	-0.7885642	0.0166061	-2.00E-05	1.27E-08	-3.27E-12	-14672.238	28.801954	-97629.98

1	888356.312	-3269.6062	8.3818738	-3.03E-04	3.19E-08	-9.69E-13	-4.24E-17	7066.474	-27.506362	-97629.98
HPO										
0	-38163.1412	792.76419	-1.8899407	0.0180091	-1.86E-05	1.02E-08	-2.36E-12	-11576.412	36.929259	-56868.759
1	384245.945	-2434.9517	8.5821739	-4.06E-04	-1.67E-08	2.25E-11	-1.94E-15	5761.6321	-26.490975	-56868.759
HSO3F										
0	0	0	2.1192445	0.0315457	-3.13E-05	1.25E-08	-8.25E-13	-92361.596	15.559696	-753129.06
1	0	0	10.36419	0.0053861	-2.12E-06	3.82E-10	-2.58E-14	-94398.334	-26.005503	-753129.06
H2										
0	40783.2281	-800.91855	8.2147017	-0.0126971	1.75E-05	-1.20E-08	3.37E-12	2682.4844	-30.437887	0
1	560812.338	-837.14913	2.975363	0.0012522	-3.74E-07	5.94E-11	-3.61E-15	5339.8159	-2.2027641	0
2	4.97E+08	-314744.81	79.838875	-0.0084145	4.75E-07	-1.37E-11	1.61E-16	2488354.7	-669.55242	0
H2+										
0	-31208.9221	230.463	3.3355612	-0.002419	7.01E-06	-5.61E-09	1.56E-12	177410.46	-0.8278338	1494672.4
1	1672226.18	-6595.1854	12.79322	-0.0055093	2.03E-06	-3.35E-10	1.95E-14	218999.96	-67.927111	1494672.4
2	-1.82E+08	101819.13	-12.458208	0.0010766	-3.93E-08	6.29E-13	-2.09E-18	-651306.16	147.14056	1494672.4
H2-										
0	0	0	3.8380142	-0.0031795	1.00E-05	-9.55E-09	3.13E-12	27234.856	-3.9986236	235376.9
1	0	0	3.2921076	0.0014359	-5.47E-07	1.04E-10	-7.38E-15	27216.181	-1.9827777	235376.9
HBOH										
0	-61596.4419	1223.483	-5.4603705	0.0355539	-4.68E-05	3.24E-08	-8.99E-12	-12636.591	54.223523	-48724.364
1	1534611.049	-5753.6664	12.708937	-7.06E-04	1.03E-07	-7.67E-12	2.21E-16	27793.704	-56.088601	-48724.364
HCHO,formaldehy										
0	-117392.211	1873.6365	-6.8903277	0.0264157	-2.19E-05	1.01E-08	-2.02E-12	-23073.555	64.204412	-108580
1	1700799.002	-7620.7867	14.72441	-0.0016491	3.29E-07	-3.49E-11	1.53E-15	31467.691	-73.864321	-108580
HCOOH										
0	-29063.3191	765.84493	-3.32845	0.0281755	-2.37E-05	1.17E-08	-2.79E-12	-50064.469	43.871135	-378570
1	487217.925	-7632.197	21.32784	-0.0044025	1.10E-06	-1.36E-10	6.65E-15	-5781.6989	-111.17878	-378570
H2F2										
0	52592.1471	-991.35449	10.435771	-0.0024078	-6.38E-07	2.74E-09	-1.10E-12	-65724.608	-30.384321	-569923.78
1	1464995.601	-3335.0749	9.187487	0.0010511	-3.28E-07	4.46E-11	-2.28E-15	-48254.421	-26.391282	-569923.78
H2O										
0	-39479.6083	575.5731	0.9317827	0.0072227	-7.34E-06	4.96E-09	-1.34E-12	-33039.743	17.242058	-241826
1	1034972.096	-2412.6986	4.6461108	0.002292	-6.84E-07	9.43E-11	-4.82E-15	-13842.865	-7.9781485	-241826
H2O+										
0	-42143.9104	675.35706	-0.0196771	0.0107169	-1.28E-05	9.21E-09	-2.65E-12	113695.27	22.936644	981600.97
1	626595.508	-2873.5517	7.7263616	-9.07E-04	6.19E-07	-1.20E-10	7.41E-15	134269.47	-26.430646	981600.97
2	-1.75E+07	-2632.7043	11.655274	-7.73E-04	5.63E-08	-1.96E-12	2.68E-17	116816.84	-57.626287	981600.97
H2O2										
0	-92795.3358	1564.7484	-5.9764601	0.0327074	-3.93E-05	2.51E-08	-6.47E-12	-24940.047	58.771742	-135880
1	1489428.027	-5170.8218	11.28205	-8.04E-05	-1.82E-08	6.95E-12	-4.83E-16	14182.51	-46.508557	-135880
H2S										
0	11970.21744	-102.89385	4.2399464	-8.02E-04	4.48E-06	-2.75E-09	4.53E-13	-3114.0347	0.3807634	-20600
1	1432316.933	-5290.9657	10.168318	-9.72E-04	2.12E-07	-2.18E-11	9.37E-16	29131.393	-43.54202	-20600
H2SO4										
0	-41291.5005	668.15899	-2.6327535	0.0541538	-7.07E-05	4.68E-08	-1.24E-11	-93156.601	39.610977	-732731.72
1	1437877.914	-6614.9025	21.576621	-4.81E-04	3.01E-08	2.33E-12	-2.95E-16	-52590.93	-102.36036	-732731.72
H2BOH										
0	-86867.6678	1820.3351	-10.323739	0.049228	-5.98E-05	3.95E-08	-1.07E-11	-44152.382	79.861773	-289633.9
1	2294795.193	-9382.9236	17.982283	-0.0015061	2.64E-07	-2.48E-11	9.74E-16	20397.39	-94.482012	-289633.9
HB(OH)2										
0	-20670.44022	953.44592	-8.0889565	0.0597243	-8.07E-05	5.61E-08	-1.55E-11	-82642.708	65.395716	-644438.72
1	2122674.609	-8615.9489	19.661795	-8.15E-04	8.96E-08	-3.34E-12	-6.92E-17	-27887.904	-99.835596	-644438.72
H3BO3										
0	25689.01843	113.80295	-4.0450966	0.0592452	-8.15E-05	5.66E-08	-1.55E-11	-122170.21	41.322201	-1004360.4
1	2297369.132	-8933.5718	21.934966	-3.09E-04	-5.06E-08	1.48E-11	-9.76E-16	-69702.985	-112.22928	-1004360.4
H3B3O3										
0	-198528.4188	4104.1321	-28.272156	0.1269639	-1.56E-04	9.97E-08	-2.60E-11	-164849.44	176.39174	-1203761
1	1286220.713	-10932.588	32.135187	-0.0025954	5.35E-07	-5.83E-11	2.60E-15	-87528.569	-177.08478	-1203761
H3B3O6										
0	-20670.31503	708.33915	-7.123821	0.102505	-1.30E-04	8.32E-08	-2.15E-11	-277804.92	60.635976	-2263687.6
1	1952433.352	-11549.329	38.926761	-0.0011139	1.28E-07	-5.73E-12	-2.21E-17	-212092.71	-207.55668	-2263687.6
H3F3										
0	98885.6265	-1380.2129	8.9804585	0.0187161	-3.13E-05	2.59E-08	-8.04E-12	-101366.15	-25.853026	-883676.79
1	2515790.373	-8789.4233	20.239334	-0.0011317	1.69E-07	-1.31E-11	3.98E-16	-54717.137	-99.077876	-883676.79
H3O+										
0	-79273.6169	1321.8864	-4.3050896	0.0230675	-2.52E-05	1.60E-08	-4.16E-12	64576.004	45.85348	598000
1	2961335.277	-9200.9969	13.428453	-5.66E-04	1.31E-08	7.05E-12	-6.03E-16	129153.94	-70.324346	598000
2	-1.59E+07	4874.1141	8.8875193	1.29E-04	-8.10E-09	2.62E-13	-3.43E-18	21097.431	-32.229972	598000
(HCOOH)2										
0	-200147.735	3502.5037	-18.535166	0.0954755	-1.06E-04	6.32E-08	-1.57E-11	-117262.39	131.96623	-820942.64
1	3308073.03	-16336.319	37.513054	-0.0031479	6.01E-07	-6.14E-11	2.60E-15	-6268.1903	-210.74461	-820942.64
H4F4										
0	131510.9024	-1840.3616	12.640932	0.0249541	-4.17E-05	3.45E-08	-1.07E-11	-136400.35	-41.229135	-1186932.3
1	3354037.99	-11719.22	27.652436	-0.0015089	2.26E-07	-1.74E-11	5.30E-16	-74202.132	-138.86033	-1186932.3
H5F5										
0	164136.1897	-2300.5104	16.301405	0.0311921	-5.21E-05	4.32E-08	-1.34E-11	-171434.54	-56.821574	-1490187.9
1	4192290.73	-14649.03	35.065549	-0.0018862	2.82E-07	-2.18E-11	6.63E-16	-93687.042	-178.8592	-1490187.9
H6F6										
0	195688.6618	-2753.9099	19.756251	0.0380772	-6.34E-05	5.22E-08	-1.61E-11	-207926.94	-71.13608	-1805545.1
1	5024520.32	-17428.179	42.148705	-0.0020846	2.93E-07	-2.05E-11	5.21E-16	-115449.77	-216.3947	-1805545.1
H7F7										
0	229386.7477	-3220.8079	23.622352	0.043668	-7.30E-05	6.04E-08	-1.88E-11	-241863.75	-88.388123	-2099699

1	5868789.83	-20508.635	49.891761	-0.0026406	3.95E-07	-3.05E-11	9.28E-16	-133017.78	-259.23851	-2099699
He										
0	0	0	2.5	0	0	0	0	-745.375	0.928724	0
1	0	0	2.5	0	0	0	0	-745.375	0.928724	0
2	3396845.42	-2194.0377	3.0802319	-8.07E-05	6.25E-09	-2.57E-13	4.43E-18	16505.19	-4.0488144	0
He+										
0	0	0	2.5	0	0	0	0	285323.37	1.6216656	2378521.5
1	0	0	2.5	0	0	0	0	285323.37	1.6216656	2378521.5
2	0	0	2.5	0	0	0	0	285323.37	1.6216656	2378521.5
Hg										
0	0	0	2.5	0	0	0	0	6636.9001	6.8002015	61380
1	51465.7351	-168.12699	2.7183431	-1.45E-04	5.16E-08	-9.47E-12	7.03E-16	7688.6849	5.2712361	61380
2	5.36E+08	-443385.38	146.3224	-0.0231844	1.92E-06	-7.42E-11	1.07E-15	3391999.9	-1201.226	61380
Hg+										
0	4.10E-04	-4.34E-06	2.5	-4.39E-11	5.56E-14	-3.64E-17	9.61E-21	128503.75	7.4933445	1074643.1
1	-12299.84728	27.322699	2.4841822	-4.43E-06	7.49E-09	-2.55E-12	2.82E-16	128318.83	7.6252446	1074643.1
2	-5.50E+07	37755.435	-7.1555456	0.0011703	-7.93E-08	4.03E-12	-7.74E-17	-167689.42	91.1675	1074643.1
HgBr2										
0	0	0	6.7188921	0.0025783	-2.92E-06	9.58E-10	1.39E-13	-12371.434	-0.4136708	-85451.725
1	0	0	7.422699	7.87E-05	-2.99E-08	4.85E-12	-2.79E-16	-12522.02	-3.8673397	-85451.725
I										
0	169.8199675	-2.7164372	2.5173856	-5.73E-05	1.03E-07	-9.67E-11	3.71E-14	12107.501	7.4058231	106760
1	-778586.057	2303.2796	0.0028867	0.0011809	-2.26E-07	1.96E-11	-6.24E-16	-2616.7927	25.58923	106760
2	4.75E+07	-86811.112	39.50617	-0.0065141	5.38E-07	-1.97E-11	2.64E-16	638484.3	-297.29971	106760
I+										
0	-801.496901	8.1390526	2.4701748	4.16E-05	7.13E-09	-7.11E-11	4.87E-14	134079.42	7.9034201	1121351
1	-778838.533	2404.9627	-0.1791751	0.0012273	-1.80E-07	9.92E-12	-9.78E-17	118853.16	27.105443	1121351
2	-6.31E+08	397113.19	-98.60192	0.0135824	-9.92E-07	3.68E-11	-5.30E-16	-3001474.6	879.04687	1121351
I-										
0	0	0	2.5	0	0	0	0	-24149.709	6.1134654	-194595.57
1	0	0	2.5	0	0	0	0	-24149.709	6.1134654	-194595.57
2	0	0	2.5	0	0	0	0	-24149.709	6.1134654	-194595.57
IF5										
0	202611.38	-3598.0827	25.302942	-0.0134845	1.11E-05	-4.71E-09	7.86E-13	-87001.954	-111.26891	-841000
1	-362191.846	-163.53624	16.122315	-4.89E-05	1.08E-08	-1.24E-12	5.72E-17	-106166.73	-53.984761	-841000
IF7										
0	299966.92	-5501.2923	36.269896	-0.0209537	1.76E-05	-7.82E-09	1.40E-12	-93314.333	-175.41358	-961500
1	-561476.595	-264.54064	22.198717	-7.98E-05	1.77E-08	-2.03E-12	9.42E-17	-122525.11	-87.739502	-961500
I2										
0	-5087.96877	-12.495852	4.5042191	1.37E-04	-1.39E-07	1.17E-10	-2.34E-14	6213.4698	5.5838369	62420
1	-5632594.16	17939.616	-17.230552	0.0124421	-3.33E-06	4.13E-10	-1.96E-14	-106850.53	160.05319	62420
In										
0	51495.1805	-917.7999	8.938688	-0.0222411	3.82E-05	-2.89E-08	8.05E-12	32390.316	-27.64567	240700
1	-1683608.899	2210.4732	3.4722194	-0.0010823	3.48E-07	-5.16E-11	3.18E-15	10959.652	2.5571891	240700
2	-2289146.601	39086.911	-17.892049	0.0036554	-2.58E-07	7.93E-12	-9.07E-17	-237625.75	173.80486	240700
In+										
0	0.215048891	-0.0025239	2.5000119	-2.87E-08	3.75E-11	-2.53E-14	6.84E-18	96.109302	5.9632544	6996.425
1	45369.9514	-144.51421	2.6818124	-1.16E-04	3.95E-08	-6.88E-12	4.82E-16	1004.2614	4.6837592	6996.425
2	-6.19E+07	13226.403	7.4533038	-0.0018933	2.11E-07	-8.43E-12	1.19E-16	-133585.9	-27.658704	6996.425
InBr										
0	-2540.851435	-52.947047	4.7174381	-4.34E-04	6.51E-07	-4.40E-10	1.23E-13	-7607.5943	4.258881	-54115.879
1	794837.442	-2318.1837	7.0328896	-0.0012459	3.28E-07	-3.00E-11	5.85E-16	6957.6273	-12.735027	-54115.879
InBr2										
0	-66.198789	-236.58973	7.9265452	-0.0019945	2.42E-06	-1.55E-09	4.06E-13	-18953.556	-5.3388675	-149729.06
1	-321716.203	479.26821	7.1026495	-5.51E-04	3.16E-07	-5.51E-11	3.17E-15	-23709.237	0.1193263	-149729.06
InBr3										
0	-4990.1153	-280.59305	11.103561	-0.00238	2.89E-06	-1.84E-09	4.81E-13	-32505.049	-18.71749	-256587.27
1	-35057.831	-4.8587213	10.004061	-1.77E-06	4.16E-10	-5.02E-14	2.42E-18	-33931.792	-12.290699	-256587.27
InCL										
0	6430.71303	-217.82677	5.4188309	-0.002048	2.70E-06	-1.80E-09	4.85E-13	-8959.8411	-1.2030022	-72147.883
1	-274575.1636	894.09869	3.2681184	9.18E-04	-3.08E-07	5.75E-11	-3.65E-15	-15616.034	12.668801	-72147.883
InCL2										
0	9935.16487	-417.21019	8.5884949	-0.0033484	4.00E-06	-2.53E-09	6.54E-13	-24264.803	-11.645222	-201483.42
1	-332871.984	475.76916	7.1054437	-5.53E-04	3.16E-07	-5.51E-11	3.17E-15	-29950.959	-2.2945604	-201483.42
InCL3										
0	26147.43044	-841.46046	13.117848	-0.0064353	7.55E-06	-4.71E-09	1.20E-12	-43264.696	-35.000816	-369693.23
1	-71140.4363	-16.284251	10.013096	-5.54E-06	1.28E-09	-1.52E-13	7.23E-18	-47589.742	-16.697616	-369693.23
InF										
0	31901.2332	-529.52543	6.1728863	-0.002986	3.23E-06	-1.86E-09	4.47E-13	-21871.763	-7.5912166	-193419.99
1	-468900.12	1321.0191	2.8813294	0.0010416	-3.09E-07	4.93E-11	-2.70E-15	-33083.698	13.966883	-193419.99
InF2										
0	75224.8021	-1088.6169	9.4817052	-0.0028932	1.52E-06	-7.99E-11	-1.47E-13	-51243.362	-21.466661	-457186.82
1	431896.034	-1688.4724	8.925863	-0.0010492	2.72E-07	-2.88E-11	1.07E-15	-46736.919	-19.324644	-457186.82
InF3										
0	107160.8336	-1660.0719	13.959728	-0.0050187	3.23E-06	-7.82E-10	-3.73E-14	-97952.15	-46.063535	-863079.57
1	-165685.5506	-79.658893	10.059133	-2.35E-05	5.16E-09	-5.89E-13	2.72E-17	-106868.26	-21.329682	-863079.57
InH										
0	-51528.2872	781.37926	-0.8433385	0.0104447	-9.76E-06	4.54E-09	-8.17E-13	21100.489	29.393462	215016.9
1	779740.666	-3646.8821	9.5429674	-0.0034813	1.30E-06	-2.18E-10	1.27E-14	46432.955	-36.593292	215016.9
InI										
0	-468.634874	-56.85531	4.7818497	-6.62E-04	1.03E-06	-7.27E-10	2.08E-13	2095.5703	4.8855151	26417.124
1	1529221.772	-4690.3737	10.045935	-0.0031404	9.46E-07	-1.25E-10	5.95E-15	31524.781	-32.976975	26417.124

InI2										
0	-4513.8906	-118.37269	7.4731101	-0.0010345	1.27E-06	-8.23E-10	2.18E-13	-6278.536	-0.6667298	-39460.643
1	-313067.1665	481.38107	7.1009142	-5.51E-04	3.16E-07	-5.51E-11	3.17E-15	-10430.128	2.1416623	-39460.643
InI3										
0	-8728.39717	-126.59149	10.506591	-0.0011061	1.35E-06	-8.71E-10	2.29E-13	-15082.691	-12.114117	-105435.91
1	-21967.42567	-2.1511675	10.001822	-8.00E-07	1.90E-10	-2.30E-14	1.11E-18	-15724.063	-9.1708887	-105435.91
InO										
0	-115472.7169	1753.6687	-6.9650338	0.029617	-3.12E-05	1.44E-08	-2.24E-12	8188.6796	66.086213	145993.11
1	-805213.095	1693.0642	4.7608636	-7.34E-04	3.23E-07	-4.58E-11	1.95E-15	4005.5198	3.5007425	145993.11
InOH										
0	61234.6302	-1195.8631	10.41428	-0.00687	6.21E-06	-2.41E-09	3.18E-13	-10798.522	-31.898908	-124447.34
1	852512.893	-2350.3172	7.9845151	9.92E-05	-6.21E-08	1.02E-11	-5.68E-16	-1536.2136	-20.431076	-124447.34
In2Br2										
0	-9221.1883	-36.16677	10.147288	-3.26E-04	4.02E-07	-2.60E-10	6.87E-14	-26448.835	-10.003601	-196305.22
1	-12907.81804	-0.6075401	10.000522	-2.31E-07	5.52E-11	-6.71E-15	3.25E-19	-26631.369	-9.1499495	-196305.22
In2Br4										
0	-14255.55379	-286.60093	17.138663	-0.0024735	3.02E-06	-1.93E-09	5.07E-13	-55937.531	-38.37106	-436508.68
1	-44534.6371	-4.911524	16.004138	-1.81E-06	4.28E-10	-5.17E-14	2.50E-18	-57391.754	-31.749064	-436508.68
In2Br6										
0	-17589.40752	-485.90345	23.916545	-0.0041421	5.03E-06	-3.22E-09	8.41E-13	-79888.445	-64.378719	-628683.43
1	-69450.3948	-8.4023682	22.007039	-3.07E-06	7.24E-10	-8.72E-14	4.20E-18	-82357.599	-53.221928	-628683.43
In2CL2										
0	-11428.48747	-141.60158	10.568533	-0.0012443	1.53E-06	-9.83E-10	2.58E-13	-30263.271	-15.651053	-232177.38
1	-26166.06332	-2.4019555	10.00204	-8.98E-07	2.13E-10	-2.58E-14	1.25E-18	-30980.167	-12.349468	-232177.38
In2CL4										
0	9814.08308	-848.8959	19.234104	-0.0068157	8.13E-06	-5.13E-09	1.32E-12	-70276.881	-55.826662	-579125.86
1	-85037.7179	-15.524646	16.012697	-5.44E-06	1.27E-09	-1.51E-13	7.25E-18	-74619.217	-36.911511	-579125.86
In2CL6										
0	30046.63159	-1585.6214	27.964895	-0.0124551	1.48E-05	-9.25E-09	2.38E-12	-104882.83	-97.884053	-882340.03
1	-149940.0484	-29.886808	22.024254	-1.03E-05	2.40E-09	-2.86E-13	1.36E-17	-113011.02	-62.939863	-882340.03
In2F2										
0	7255.7171	-644.82657	12.475395	-0.0052461	6.28E-06	-3.97E-09	1.03E-12	-63848.925	-31.080046	-532234.3
1	-64097.1544	-11.637407	10.009565	-4.11E-06	9.61E-10	-1.15E-13	5.51E-18	-67142.779	-16.617185	-532234.3
In2F4										
0	122521.3611	-2444.9984	23.424255	-0.0129143	1.31E-05	-7.18E-09	1.65E-12	-146694.21	-89.435601	-1284788.1
1	-220597.7486	-78.220838	16.059239	-2.39E-05	5.33E-09	-6.14E-13	2.86E-17	-159571.63	-44.695746	-1284788.1
In2F6										
0	182549.0583	-3552.1117	32.754252	-0.0186806	1.89E-05	-1.04E-08	2.39E-12	-223964.88	-136.36268	-1960000
1	-317096.638	-116.7441	22.088475	-3.58E-05	7.97E-09	-9.19E-13	4.28E-17	-242666.11	-71.553286	-1960000
In2I2										
0	-6681.92501	-14.491032	10.059291	-1.31E-04	1.63E-07	-1.06E-10	2.79E-14	-6279.6026	-7.291131	-27813.524
1	-8148.1573	-0.2444544	10.000211	-9.38E-08	2.24E-11	-2.73E-15	1.33E-19	-6352.6515	-6.9477254	-27813.524
In2I4										
0	-15010.28064	-97.447979	16.39384	-8.66E-04	1.07E-06	-6.88E-10	1.81E-13	-28303.884	-29.862948	-199143.18
1	-25056.99251	-1.6421552	16.001401	-6.19E-07	1.47E-10	-1.79E-14	8.65E-19	-28796.553	-27.577904	-199143.18
In2I6										
0	-22326.40607	-200.07869	22.804179	-0.0017613	2.16E-06	-1.39E-09	3.66E-13	-44125.477	-52.73802	-319720.04
1	-43119.0585	-3.3903506	22.002881	-1.27E-06	3.01E-10	-3.65E-14	1.77E-18	-45138.203	-48.068684	-319720.04
In2O										
0	50656.535	-807.03637	8.6420673	-0.001533	2.87E-07	4.98E-10	-2.55E-13	-1924.9085	-14.907188	-34763.707
1	-92327.8636	-52.011273	7.0387236	-1.54E-05	3.40E-09	-3.89E-13	1.80E-17	-6270.9268	-4.4218204	-34763.707
K										
0	9.66514393	-0.1458059	2.5008659	-2.60E-06	4.19E-09	-3.44E-12	1.13E-15	9959.4935	5.0358223	89000
1	-3566422.36	10852.898	-10.541349	0.0080098	-2.70E-06	4.72E-10	-2.98E-14	-58753.37	97.385512	89000
2	9.21E+08	-693530.03	191.12708	-0.0230593	1.43E-06	-4.41E-11	5.37E-16	5395082.2	-1622.1588	89000
K+										
0	0	0	2.5	0	0	0	0	61075.169	4.3474044	514007.53
1	0	0	2.5	0	0	0	0	61075.169	4.3474044	514007.53
2	2.18E+07	-14150.766	6.2489543	-5.19E-04	3.96E-08	-1.58E-12	2.60E-17	172275.36	-27.81729	514007.53
K-										
0	0	0	2.5	0	0	0	0	3394.1507	4.3474465	34418.128
1	0	0	2.5	0	0	0	0	3394.1507	4.3474465	34418.128
2	0	0	2.5	0	0	0	0	3394.1507	4.3474465	34418.128
KBO2										
0	0	0	4.3967801	0.0121692	-1.18E-05	5.13E-09	-6.59E-13	-82827.012	7.5732431	-674054.74
1	0	0	7.5502508	0.0025662	-1.07E-06	1.99E-10	-1.37E-14	-83653.834	-8.4927	-674054.74
KCN										
0	0	0	5.0810711	0.0055266	-9.12E-06	8.45E-09	-3.01E-12	7866.2161	0.186333	79499.339
1	0	0	5.800712	0.0017201	-7.08E-07	1.32E-10	-9.19E-15	7727.2628	-3.158848	79499.339
KCL										
0	0	0	3.9908569	0.0021089	-3.18E-06	2.25E-09	-5.91E-13	-27080.184	5.5120045	-214685.06
1	0	0	4.4636733	1.22E-04	-9.17E-09	9.26E-13	-1.04E-17	-27173.133	3.24809	-214685.06
KF										
0	0	0	3.5156066	0.0037868	-5.59E-06	3.78E-09	-9.39E-13	-40476.079	6.3133855	-326776.27
1	0	0	4.40407	1.78E-04	-3.61E-08	5.88E-12	-3.47E-16	-40655.889	2.0310959	-326776.27
KF2-										
0	0	0	5.2507573	0.0086384	-1.34E-05	9.41E-09	-2.47E-12	-85383.971	-0.4772247	-694556.68
1	0	0	7.2581638	2.67E-04	-1.14E-07	2.14E-11	-1.48E-15	-85780.839	-10.103278	-694556.68
KH										
0	0	0	2.8157756	0.0039871	-3.34E-06	8.86E-10	1.14E-13	13805.838	6.725179	123012.03
1	0	0	3.9603386	7.22E-04	-2.69E-07	5.26E-11	-3.79E-15	13501.837	0.8553451	123012.03
KO										

0	0	0	3.7410778	0.0031242	-4.80E-06	3.47E-09	-9.36E-13	7336.8714	6.5669239	71131.606
1	0	0	4.4244778	1.99E-04	-3.71E-08	7.13E-12	-5.04E-16	7205.2331	3.3076685	71131.606
KO-										
0	0	0	3.708366	0.0032376	-4.97E-06	3.57E-09	-9.61E-13	-17818.607	5.3166259	-138073.65
1	0	0	4.4201084	2.01E-04	-3.93E-08	7.56E-12	-5.34E-16	-17956.109	1.9200041	-138073.65
KOH										
0	17706.84196	-615.32052	8.6840757	-0.0039628	3.41E-06	-9.60E-10	8.49E-15	-26779.033	-21.744957	-232000
1	891727.195	-2334.1791	7.9725787	1.04E-04	-6.32E-08	1.03E-11	-5.74E-16	-14436.965	-20.764014	-232000
KOH+										
0	0	0	4.4325167	0.0084632	-1.42E-05	1.11E-08	-3.16E-12	58292.632	2.8733457	497913.83
1	0	0	5.680614	0.0012121	-3.34E-07	4.17E-11	-1.88E-15	58167.602	-2.5541514	497913.83
K2										
0	19500.2553	-396.25241	7.4803064	-0.0110787	2.25E-05	-2.10E-08	6.84E-12	15298.901	-11.333519	123672.13
1	-4205896.42	11705.709	-5.4923802	0.002863	-5.70E-07	5.95E-11	-2.54E-15	-62729.196	80.551743	123672.13
K2C2N2										
0	0	0	11.133058	0.0115164	-1.95E-05	1.82E-08	-6.46E-12	-4698.0693	-21.267973	-8365.237
1	0	0	12.625754	0.0034124	-1.40E-06	2.62E-10	-1.82E-14	-4975.3614	-28.153905	-8365.237
K2CL2										
0	0	0	8.7067974	0.0060154	-1.13E-05	9.66E-09	-3.11E-12	-77067.696	-8.5375473	-617657.01
1	0	0	9.9041069	1.12E-04	-5.04E-08	9.99E-12	-7.27E-16	-77272.33	-14.090282	-617657.01
K2F2										
0	0	0	7.8329504	0.0089241	-1.47E-05	1.10E-08	-3.07E-12	-106387.52	-8.2423828	-862757.41
1	0	0	9.8148096	2.05E-04	-8.71E-08	1.63E-11	-1.13E-15	-106759.87	-17.641803	-862757.41
K2O2H2										
0	8174.78837	-1130.6307	18.153033	-0.0077374	6.84E-06	-2.05E-09	7.67E-14	-75749.652	-63.917595	-641000
1	1773523.196	-4665.2925	16.943081	2.09E-04	-1.26E-07	2.06E-11	-1.15E-15	-50512.633	-63.347739	-641000
K2SO4										
0	0	0	3.475852	0.0487732	-6.84E-05	4.69E-08	-1.27E-11	-134280.85	12.344829	-1094144.1
1	0	0	15.374108	0.0041056	-1.81E-06	3.55E-10	-2.56E-14	-136953.29	-46.143815	-1094144.1
Kr										
0	0	0	2.5	0	0	0	0	-745.375	5.4909565	0
1	264.3639057	-0.7910051	2.5009206	-5.33E-07	1.62E-10	-2.47E-14	1.48E-18	-740.34889	5.4843982	0
2	-1.38E+09	906403.05	-240.34814	0.0337831	-2.56E-06	9.97E-11	-1.52E-15	-7111667.4	2086.8663	0
Kr+										
0	-5650.40286	69.307408	2.1570281	8.71E-04	-1.18E-06	7.86E-10	-1.83E-13	162116.41	8.8182423	1356953.9
1	-221656.7015	1166.1678	0.4869655	0.0014292	-3.95E-07	4.98E-11	-2.41E-15	155600.29	20.59231	1356953.9
2	-3.32E+07	17979.531	-0.7155016	2.67E-04	-6.20E-09	-4.11E-13	2.00E-17	16481.143	36.203258	1356953.9
Li										
0	0	0	2.5	0	0	0	0	18413.902	2.447623	159300
1	1125610.652	-3463.5367	6.5666119	-0.002261	5.92E-07	-6.28E-11	2.88E-15	40346.374	-26.559182	159300
2	2.60E+09	-1521952.2	345.44005	-0.0377967	2.22E-06	-6.69E-11	8.09E-16	1.22E+07	-3006.6802	159300
Li+										
0	0	0	2.5	0	0	0	0	81727.246	1.7543572	685719.43
1	0	0	2.5	0	0	0	0	81727.246	1.7543572	685719.43
2	0	0	2.5	0	0	0	0	81727.246	1.7543572	685719.43
Li-										
0	0	0	2.5	0	0	0	0	10496.987	1.7545943	93474.728
1	0	0	2.5	0	0	0	0	10496.987	1.7545943	93474.728
2	0	0	2.5	0	0	0	0	10496.987	1.7545943	93474.728
LiALF4										
0	0	0	2.5403421	0.0519859	-8.62E-05	6.75E-08	-2.04E-11	-225357.67	12.571932	-1853531.7
1	0	0	14.037742	0.0022483	-1.00E-06	1.97E-10	-1.42E-14	-227627.57	-42.360148	-1853531.7
LiBO2										
0	0	0	3.7435474	0.0144753	-1.52E-05	7.41E-09	-1.22E-12	-79437.756	8.0120256	-646856.75
1	0	0	7.4266096	0.0027044	-1.13E-06	2.11E-10	-1.46E-14	-80370.285	-10.600792	-646856.75
LiCL										
0	0	0	2.9906906	0.0050339	-6.57E-06	3.81E-09	-7.61E-13	-24603.182	7.3281845	-195712.17
1	0	0	4.2712143	3.14E-04	-1.01E-07	1.85E-11	-1.24E-15	-24884.442	1.0417216	-195712.17
LiF										
0	0	0	2.8528869	0.0039533	-3.17E-06	4.32E-10	3.71E-13	-41987.265	6.7910289	-340794.85
1	0	0	4.0430248	5.70E-04	-2.15E-07	4.06E-11	-2.84E-15	-42299.318	0.6976955	-340794.85
LiFO										
0	0	0	2.500179	0.0126617	-1.42E-05	6.45E-09	-7.43E-13	-12265.534	12.144018	-92041.76
1	0	0	5.9926109	0.0011139	-4.79E-07	9.11E-11	-6.38E-15	-13100.989	-5.3366033	-92041.76
LiF2-										
0	0	0	3.4718136	0.0106367	-1.18E-05	5.68E-09	-8.47E-13	-86963.111	5.140928	-711293.51
1	0	0	6.344859	0.0012571	-5.35E-07	1.01E-10	-7.06E-15	-87667.89	-9.2984029	-711293.51
LiH										
0	0	0	3.4209486	-6.81E-04	5.65E-06	-6.22E-09	2.15E-12	15884.945	1.0657419	140625.95
1	0	0	3.5884297	0.0010728	-4.02E-07	7.38E-11	-4.93E-15	15717.625	-0.375039	140625.95
LiN										
0	0	0	2.88943	0.0052213	-6.60E-06	3.73E-09	-7.24E-13	39216.323	7.2888715	334730.69
1	0	0	4.2258077	3.97E-04	-1.25E-07	2.32E-11	-1.59E-15	38916.952	0.7008515	334730.69
LiO										
0	0	0	2.8389007	0.0051539	-6.31E-06	3.41E-09	-6.16E-13	9088.4314	7.9131179	84098.28
1	0	0	4.1876205	4.12E-04	-1.45E-07	2.73E-11	-1.89E-15	8779.5259	1.231426	84098.28
LiO-										
0	0	0	2.8515866	0.005017	-5.95E-06	3.04E-09	-4.79E-13	-9077.8076	6.4594707	-66943.828
1	0	0	4.1810217	4.18E-04	-1.50E-07	2.84E-11	-1.98E-15	-9384.9702	-0.1423923	-66943.828
LiOH										
0	4573.91725	-103.09121	4.2723881	0.0084653	-1.39E-05	1.10E-08	-3.29E-12	-28487.306	-0.8774661	-229000
1	850066.921	-2430.5197	8.0552938	6.90E-05	-5.53E-08	9.37E-12	-5.31E-16	-13659.081	-24.575829	-229000

LiOH+										
0	0	0	3.6379739	0.0108972	-1.72E-05	1.27E-08	-3.42E-12	92161.193	3.6377609	778249.76
1	0	0	5.5329269	0.0013778	-4.07E-07	5.56E-11	-2.86E-15	91888.579	-4.9935927	778249.76
LiON										
0	0	0	3.6701164	0.0072568	-5.87E-06	1.16E-09	4.27E-13	20271.703	6.6824951	179918.9
1	0	0	5.8123496	0.0012871	-5.47E-07	1.03E-10	-7.19E-15	19692.302	-4.3447056	179918.9
Li2										
0	6778.48655	-224.62066	5.2960379	-0.0012724	1.21E-06	-9.82E-11	-2.42E-13	25736.382	-6.86926	215900
1	3.77E+07	-118574.71	148.21677	-0.0837853	2.42E-05	-3.28E-09	1.65E-13	772307.17	-1021.6973	215900
Li2CL2										
0	0	0	5.2801351	0.0183841	-2.88E-05	2.03E-08	-5.34E-12	-74160.003	0.2792794	-598521.42
1	0	0	9.5245614	5.25E-04	-2.23E-07	4.20E-11	-2.90E-15	-74990.263	-20.031672	-598521.42
Li2F2										
0	0	0	2.4007508	0.0270662	-3.93E-05	2.57E-08	-6.22E-12	-115010.91	10.891779	-942791
1	0	0	8.9566636	0.0011719	-5.10E-07	9.79E-11	-6.92E-15	-116372.28	-20.886331	-942791
Li2O										
0	0	0	3.9721708	0.0092461	-9.36E-06	3.46E-09	-7.57E-14	-21596.988	2.5523041	-166935.47
1	0	0	6.6198748	9.69E-04	-4.15E-07	7.86E-11	-5.50E-15	-22255.325	-10.821559	-166935.47
Li2O2										
0	0	0	5.5375232	0.0173442	-2.72E-05	1.93E-08	-5.12E-12	-31402.044	-2.7683129	-242656.43
1	0	0	9.527526	5.30E-04	-2.30E-07	4.40E-11	-3.10E-15	-32182.484	-21.859112	-242656.43
Li2O2H2										
0	189441.9736	-2779.1269	15.302404	0.0107072	-2.51E-05	2.22E-08	-6.95E-12	-77027.725	-65.141474	-737000
1	1215363.488	-3982.0207	15.858737	7.51E-04	-2.59E-07	3.65E-11	-1.90E-15	-67387.722	-66.471816	-737000
Li2SO4										
0	0	0	0.7114573	0.0594512	-8.64E-05	6.12E-08	-1.71E-11	-127508.42	20.380328	-1041842.1
1	0	0	14.929595	0.0046097	-2.04E-06	3.99E-10	-2.87E-14	-130635.28	-49.166491	-1041842.1
Li3CL3										
0	0	0	4.5745959	0.0397492	-5.65E-05	3.63E-08	-8.58E-12	-123533.51	4.6805966	-1004679.1
1	0	0	14.31944	0.0018854	-8.20E-07	1.57E-10	-1.11E-14	-125588.51	-42.711023	-1004679.1
Li3F3										
0	0	0	4.6413975	0.0398787	-5.72E-05	3.72E-08	-8.92E-12	-185198.52	2.1623597	-1517221
1	0	0	14.364422	0.0018285	-7.92E-07	1.52E-10	-1.07E-14	-187237.36	-45.060913	-1517221
Mg										
0	0	0	2.5	0	0	0	0	16946.588	3.6343301	147100
1	-536483.155	1973.7096	-0.3633777	0.0020718	-7.74E-07	1.36E-10	-7.77E-15	4829.1881	23.39105	147100
2	2.17E+09	-1008355.7	161.968	-0.0087901	-1.93E-08	1.73E-11	-4.23E-16	8349525.9	-1469.3553	147100
Mg+										
0	0	0	2.5	0	0	0	0	106422.34	4.3274435	891047
1	-19147.58821	48.773479	2.4576627	1.22E-05	1.90E-09	-1.58E-12	2.14E-16	106102.24	4.6464429	891047
2	4.02E+08	-228159.17	54.217457	-0.005983	3.66E-07	-1.02E-11	1.02E-16	1932464	-448.01578	891047
MgBr										
0	7361.41914	-239.57899	5.3605604	-0.0016671	1.98E-06	-1.20E-09	3.03E-13	591.56344	-1.4217712	6163.315
1	24776.04216	-641.76875	6.0199321	-0.001391	6.44E-07	-1.20E-10	7.42E-15	2824.0603	-6.2644399	6163.315
MgBr2										
0	21484.77999	-515.45289	9.2732588	-0.00347	3.92E-06	-2.38E-09	5.97E-13	-36524.439	-17.910778	-306743.22
1	-43268.9901	-12.83036	7.5100243	-4.15E-06	9.43E-10	-1.10E-13	5.20E-18	-39198.86	-7.409168	-306743.22
MgCL										
0	20439.9528	-407.21552	5.8803723	-0.0025942	2.95E-06	-1.75E-09	4.34E-13	-5851.445	-6.0235533	-54704.887
1	1041328.453	-3380.1583	8.6377755	-0.0024478	7.84E-07	-1.13E-10	5.81E-15	13271.89	-27.038031	-54704.887
MgCL+										
0	0	0	3.601223	0.0034792	-5.14E-06	3.44E-09	-8.38E-13	77314.688	6.1338593	652722.9
1	0	0	6.3512344	-0.0037967	2.47E-06	-5.08E-10	3.37E-14	76480.879	-8.2903623	652722.9
MgCLF										
0	0	0	3.1570429	0.0164535	-3.01E-05	2.58E-08	-8.42E-12	-69891.004	10.22554	-569024
1	0	0	6.5708225	4.49E-04	-1.78E-07	3.06E-11	-1.92E-15	-70523.598	-5.8355541	-569024
MgCL2										
0	36378.2468	-730.7845	9.6610305	-0.0036602	3.61E-06	-1.93E-09	4.31E-13	-46469.146	-23.601132	-399169.9
1	-68352.1701	-24.908994	7.5187832	-7.56E-06	1.68E-09	-1.93E-13	8.97E-18	-50326.869	-10.532693	-399169.9
MgF										
0	38230.0162	-480.33104	5.0684689	5.21E-04	-1.87E-06	1.76E-09	-5.61E-13	-26591.143	-3.7689692	-232266.79
1	-169588.3782	358.87576	3.9360017	4.81E-04	-1.66E-07	3.34E-11	-2.27E-15	-31693.24	4.4105659	-232266.79
MgF+										
0	0	0	3.4387654	0.0022253	-5.46E-06	1.41E-08	-8.07E-12	60515.666	5.7783546	512303.56
1	0	0	4.3681057	0.0041176	-2.94E-06	7.27E-10	-5.98E-14	59536	-1.3457779	512303.56
MgF2										
0	43384.2955	-661.65118	7.4534485	0.0035208	-6.96E-06	5.62E-09	-1.69E-12	-86871.837	-15.454768	-735498.06
1	-124441.9584	-86.873438	7.5635812	-2.50E-05	5.44E-09	-6.16E-13	2.82E-17	-90600.194	-14.20797	-735498.06
MgF2+										
0	0	0	3.5212884	0.0152696	-2.52E-05	1.96E-08	-5.91E-12	69658.388	7.3902095	591997.23
1	0	0	6.8910673	7.18E-04	-3.29E-07	6.59E-11	-4.59E-15	68993.145	-8.713014	591997.23
MgH										
0	-49586.7915	750.02787	-0.6442048	0.0098263	-8.79E-06	3.82E-09	-6.00E-13	23022.794	26.571653	229786.1
1	-100574.8598	1952.8901	-1.3171915	0.0056037	-2.14E-06	3.32E-10	-1.82E-14	15985.828	34.312332	229786.1
MgI										
0	2943.889099	-169.02486	5.1472518	-0.0013212	1.62E-06	-1.01E-09	2.57E-13	6845.8903	0.8593132	61206.317
1	-2370562.811	6916.4525	-3.1838945	0.0040516	-9.77E-07	1.02E-10	-3.79E-15	-38185.511	59.931044	61206.317
MgI2										
0	15947.39709	-416.04127	9.0106383	-0.0030904	3.62E-06	-2.26E-09	5.81E-13	-20804.414	-14.121757	-171706.03
1	-33402.9918	-9.3435118	7.5074685	-3.15E-06	7.24E-10	-8.57E-14	4.07E-18	-22945.555	-5.2412726	-171706.03
MgN										
0	0	0	2.8894549	0.0051757	-6.58E-06	3.72E-09	-7.23E-13	33681.058	9.2975895	288691.68

1	0	0	4.2214417	3.65E-04	-1.30E-07	2.44E-11	-1.69E-15	33382.931	2.732052	288691.68
MgO										
0	351365.974	-5287.1972	33.820601	-0.0840049	1.21E-04	-7.63E-08	1.70E-11	27906.795	-162.48862	32261.307
1	-1.59E+07	34204.681	-17.740877	0.007005	-1.10E-06	8.96E-11	-3.05E-15	-230050.44	173.89845	32261.307
2	2290059.05	-20734.996	14.4415	-0.0014906	1.05E-07	-3.52E-12	4.61E-17	149021.88	-80.072817	32261.307
MgOH										
0	38398.5162	-736.73836	7.9206645	-5.95E-04	-2.11E-06	3.23E-09	-1.21E-12	-13923.262	-19.160781	-132428.98
1	664866.475	-1770.7504	7.2699993	5.34E-04	-1.98E-07	3.03E-11	-1.55E-15	-6149.1146	-16.71027	-132428.98
MgOH+										
0	0	0	1.7831421	0.0192285	-3.35E-05	2.75E-08	-8.52E-12	69150.584	11.930524	584436.76
1	0	0	5.2824479	0.001664	-5.40E-07	8.35E-11	-5.00E-15	68595.816	-4.1503886	584436.76
Mg(OH)2										
0	52458.9467	-1289.0564	13.893276	-7.81E-04	-4.15E-06	6.11E-09	-2.27E-12	-62950.892	-50.153533	-551995.81
1	1713709.254	-4730.0054	14.48926	1.91E-04	-1.23E-07	2.02E-11	-1.13E-15	-38877.247	-58.404981	-551995.81
MgS										
0	-9565.78809	144.36378	1.8137947	0.0114717	-2.22E-05	2.00E-08	-6.09E-12	12765.015	14.613358	120649.31
1	2.65E+07	-77113.559	84.637717	-0.0364425	8.40E-06	-9.54E-10	4.26E-14	507893.12	-583.46558	120649.31
Mg2										
0	4545.19559	411.585	0.4841196	0.004892	-6.40E-06	4.30E-09	-1.16E-12	31816.418	26.404321	286513.32
1	30382.24994	59.452405	2.3527067	1.38E-04	-5.90E-08	1.10E-11	-6.56E-16	33510.366	15.881774	286513.32
Mg2F4										
0	0	0	4.2299053	0.0492908	-8.64E-05	7.05E-08	-2.19E-11	-209492.99	5.0032362	-1718408.7
1	0	0	14.672016	0.0015299	-6.83E-07	1.35E-10	-9.74E-15	-211437.66	-44.278244	-1718408.7
Mn										
0	0.103406136	-0.0015515	2.5000091	-2.72E-08	4.33E-11	-3.51E-14	1.14E-17	33219.352	6.6493255	282400
1	5855.15582	883.85884	-0.0364866	0.0027037	-1.32E-06	2.87E-10	-1.92E-14	28678.035	22.925412	282400
2	3.94E+09	-2353549.7	537.72448	-0.0582481	3.33E-06	-9.69E-11	1.13E-15	1.88E+07	-4690.0979	282400
Mn+										
0	345.80177	-4.2511513	2.521281	-5.57E-05	8.04E-08	-6.09E-11	1.90E-14	120253.36	6.6834682	1005871.3
1	647131.41	-2403.7963	5.9377158	-0.002341	7.46E-07	-9.08E-11	4.47E-15	134990.21	-17.026663	1005871.3
2	1.72E+09	-902918.58	178.47888	-0.0156677	7.35E-07	-1.75E-11	1.67E-16	7443546.1	-1568.0058	1005871.3
Mo										
0	76.4636791	-1.159269	2.5069295	-2.10E-05	3.41E-08	-2.84E-11	9.49E-15	78458.998	7.6018357	658500
1	5573271	-16623.658	21.351471	-0.0100307	2.41E-06	-1.81E-10	1.03E-15	184264.65	-127.53264	658500
2	6.21E+09	-3855961.6	937.15951	-0.1108165	6.93E-06	-2.20E-10	2.80E-15	3.06E+07	-8122.8113	658500
Mo+										
0	129.8236623	-1.5602799	2.5076003	-1.92E-05	2.67E-08	-1.94E-11	5.73E-15	161510.38	7.4425435	1349012.9
1	1.30E+07	-39482.762	48.665998	-0.0260535	7.22E-06	-8.72E-10	3.79E-14	411894.86	-321.6791	1349012.9
2	-1.73E+09	877668.52	-166.97168	0.0173244	-9.37E-07	2.59E-11	-2.91E-16	-6989098.1	1517.1018	1349012.9
Mo-										
0	0	0	2.5	0	0	0	0	69051.237	7.4856595	580324.63
1	0	0	2.5	0	0	0	0	69051.237	7.4856595	580324.63
2	0	0	2.5	0	0	0	0	69051.237	7.4856595	580324.63
MoO3										
0	0	0	3.6543121	0.014491	-7.67E-06	-6.10E-09	5.18E-12	-45483.094	8.5052189	-364414.34
1	0	0	8.5599079	0.0015137	-6.14E-07	1.08E-10	-6.23E-15	-46765.27	-16.702825	-364414.34
Mo2O6										
0	0	0	7.7546721	0.0326251	-1.67E-05	-1.50E-08	1.24E-11	-141833.38	-6.4509273	-1149456.6
1	0	0	13.923332	0.0129087	-7.39E-06	1.75E-09	-1.44E-13	-142928.31	-36.448614	-1149456.6
Mo3O9										
0	0	0	13.577424	0.0453893	-2.13E-05	-2.29E-08	1.78E-11	-234596.88	-28.577139	-1902048.7
1	0	0	22.262299	0.018585	-1.06E-05	2.49E-09	-2.05E-13	-236200.38	-71.088186	-1902048.7
Mo4O12										
0	0	0	18.727478	0.0611595	-2.91E-05	-3.07E-08	2.40E-11	-323765.94	-50.088384	-2625550.2
1	0	0	30.431747	0.0247326	-1.41E-05	3.33E-09	-2.74E-13	-325903.63	-107.28034	-2625550.2
Mo5O15										
0	0	0	23.887054	0.076141	-3.52E-05	-3.99E-08	3.06E-11	-410521.06	-71.604177	-3329138.6
1	0	0	38.622543	0.0307427	-1.75E-05	4.13E-09	-3.41E-13	-413241.56	-143.73676	-3329138.6
N										
0	0	0	2.5	0	0	0	0	56104.638	4.1939093	472680
1	88765.0138	-107.12315	2.3621883	2.92E-04	-1.73E-07	4.01E-11	-2.68E-15	56973.513	4.8652358	472680
2	5.48E+08	-310757.5	69.167827	-0.006848	3.83E-07	-1.10E-11	1.28E-16	2550585.6	-584.87697	472680
N+										
0	5237.07921	2.2999583	2.4874888	2.74E-05	-3.13E-08	1.85E-11	-4.45E-15	225628.47	5.0768351	1882127.6
1	290497.0374	-855.79086	3.4773893	-5.29E-04	1.35E-07	-1.39E-11	5.05E-16	231081	-1.9941423	1882127.6
2	1.65E+07	-11131.652	4.9769866	-2.01E-04	1.02E-08	-2.69E-13	3.54E-18	313628.47	-17.06646	1882127.6
N-										
0	1428.934638	7.5206871	2.4758588	4.42E-05	-4.66E-08	2.64E-11	-6.21E-15	56175.317	5.1505028	473537.55
1	2051.106014	1.6353874	2.4979363	1.27E-06	-3.97E-10	5.95E-14	-3.42E-18	56205.9	5.0194328	473537.55
2	2199.831428	0.7682241	2.4995112	1.35E-07	-1.82E-11	1.11E-15	-2.42E-20	56210.924	5.0087165	473537.55
NCO										
0	9507.96917	-195.73299	4.2351279	0.0039037	3.86E-07	-2.85E-09	1.23E-12	15569.626	2.0425034	131843.93
1	73929.2978	-1617.2584	8.5749195	-3.76E-04	7.04E-08	-6.69E-12	2.99E-16	22894.071	-25.52768	131843.93
ND										
0	0	0	3.7206488	-0.0015342	3.19E-06	-1.51E-09	9.71E-14	44072.756	1.6495567	375309.26
1	0	0	2.8297034	0.0016584	-6.33E-07	1.15E-10	-7.83E-15	44255.951	6.0066288	375309.26
ND2										
0	0	0	4.026978	-0.0014085	7.78E-06	-6.50E-09	1.76E-12	21098.028	1.754843	185353.4
1	0	0	3.3515391	0.0033763	-1.32E-06	2.68E-10	-2.08E-14	21077.749	4.3738798	185353.4
ND3										
0	0	0	2.9427839	0.0051035	2.74E-06	-4.68E-09	1.63E-12	-8165.1563	6.1552204	-58576.719
1	0	0	3.1961566	0.0067312	-2.64E-06	4.76E-10	-3.28E-14	-8396.6527	4.1629072	-58576.719

NF										
0	-35049.2775	667.4503	-1.201666	0.0145207	-1.82E-05	1.16E-08	-2.97E-12	23954.14	30.892606	232990.5
1	800298.733	-3237.6966	8.7034089	-0.002701	9.15E-07	-1.37E-10	7.23E-15	46428.195	-30.199331	232990.5
NF2										
0	15118.31104	91.963899	0.4947302	0.0200185	-2.77E-05	1.87E-08	-5.02E-12	2839.2796	22.705158	34421.447
1	-194501.0078	-353.60341	7.2634944	-8.40E-05	2.33E-08	-2.67E-12	1.24E-16	3435.4406	-13.361024	34421.447
NF3										
0	87571.4928	-903.18329	4.0274173	0.0231444	-3.42E-05	2.41E-08	-6.63E-12	-12372.321	0.3026439	-131700
1	-349626.876	-497.37287	10.368661	8.90E-05	5.88E-08	-3.16E-12	1.71E-16	-17131.834	-30.989208	-131700
NH										
0	13596.5132	-190.02966	4.5184968	-0.0024328	2.38E-06	-2.59E-10	-2.66E-13	42809.722	-3.8865576	357032
1	1958141.991	-5782.8613	9.335742	-0.0022929	6.08E-07	-6.65E-11	2.38E-15	78989.123	-41.1697	357032
2	9.52E+07	-85858.269	29.804452	-0.0029796	1.66E-07	-4.74E-12	5.57E-17	696143.43	-222.90274	357032
NH+										
0	4253.65685	-245.82222	6.7089195	-0.0103849	1.51E-05	-9.58E-09	2.33E-12	200107.78	-13.950572	1665787.9
1	1405709.438	-4136.2157	7.6320145	-0.0012283	2.72E-07	-2.01E-11	3.72E-17	225897.6	-27.867848	1665787.9
2	2.39E+08	-174165.86	51.079079	-0.0055676	3.27E-07	-9.80E-12	1.19E-16	1554705.3	-406.59689	1665787.9
NHF										
0	-51106.8666	961.22922	-2.7064647	0.0203657	-2.43E-05	1.55E-08	-4.06E-12	7909.6109	40.993276	112000
1	901385.712	-3463.3878	8.7057985	-4.02E-04	2.32E-08	6.28E-12	-6.28E-16	33370.59	-29.004785	112000
NHF2										
0	-56262.0009	1205.7682	-6.0175887	0.0376004	-4.62E-05	2.94E-08	-7.60E-12	-18970.2	59.017485	-103000
1	739397.516	-4004.3847	12.213127	-6.97E-04	1.27E-07	-1.25E-11	5.09E-16	9133.6385	-48.677746	-103000
NH2										
0	-31159.71998	475.06708	1.3746162	0.0062993	-5.98E-06	4.48E-09	-1.41E-12	19291.068	15.389231	189134.66
1	1669007.546	-5610.3795	9.971875	-0.0011783	4.23E-07	-6.54E-11	3.62E-15	56890.578	-43.793534	189134.66
NH2F										
0	-109237.476	1844.9198	-7.6738716	0.0322953	-3.39E-05	1.97E-08	-4.81E-12	-18783.19	68.614839	-75000
1	1927205.34	-7500.4472	13.955896	-0.0011848	2.05E-07	-1.91E-11	7.39E-16	35529.273	-67.311853	-75000
NH3										
0	-76812.2615	1270.9516	-3.8932291	0.0214599	-2.18E-05	1.32E-08	-3.33E-12	-12648.864	43.660149	-45940
1	2452389.535	-8040.8942	12.713462	-3.98E-04	3.55E-08	2.53E-12	-3.32E-16	43861.92	-64.623303	-45940
NH4+										
0	-266831.5752	3763.0207	-15.713277	0.0454882	-4.38E-05	2.46E-08	-5.96E-12	58232.847	111.20872	644904.95
1	4141889	-14420.72	20.118936	-0.0019715	3.11E-07	-2.60E-11	8.89E-16	166419.62	-120.15357	644904.95
NO										
0	-11439.16503	153.64676	3.4314687	-0.0026686	8.48E-06	-7.69E-09	2.39E-12	9098.2144	6.7287275	91271.31
1	223901.8716	-1289.6516	5.433936	-3.66E-04	9.88E-08	-1.42E-11	9.38E-16	17503.177	-8.5016671	91271.31
2	-9.58E+08	591243.45	-138.45668	0.0169434	-1.01E-06	2.91E-11	-3.30E-16	-4677501.2	1242.0812	91271.31
NO+										
0	1398.106635	-159.04469	5.1228954	-0.0063944	1.12E-05	-7.99E-09	2.11E-12	118749.51	-4.3984318	990809.7
1	606987.69	-2278.3954	6.0803247	-6.07E-04	1.43E-07	-1.75E-11	8.94E-16	132270.96	-15.198798	990809.7
2	2.68E+09	-1832948.7	509.92494	-0.0711382	5.32E-06	-1.96E-10	2.81E-15	1.44E+07	-4324.0445	990809.7
NOCL										
0	23088.35209	-549.59838	7.7304634	-0.0050739	1.06E-05	-8.79E-09	2.65E-12	7389.8984	-13.183936	52698.828
1	-613341.333	-391.92988	9.1389172	-0.0026057	1.30E-06	-2.22E-10	1.28E-14	4517.3284	-23.073239	52698.828
NOF										
0	47550.2426	-725.39042	7.2139964	-0.0025324	6.38E-06	-5.52E-09	1.68E-12	-5609.7225	-12.896635	-65000
1	1889069.274	-6731.0227	14.190188	-0.0036931	9.94E-07	-1.08E-10	4.21E-15	32099.008	-63.702668	-65000
NOF3										
0	148840.647	-2241.1158	13.023916	0.005463	-8.64E-06	5.91E-09	-1.58E-12	-13283.109	-48.775238	-187000
1	-278621.894	-1252.1713	13.908102	-3.57E-04	7.78E-08	-8.85E-12	4.08E-16	-20257.499	-51.067777	-187000
NO2										
0	-56420.3878	963.30857	-2.434511	0.0192776	-1.87E-05	9.15E-09	-1.78E-12	-1547.925	40.678513	34193.019
1	721300.157	-3832.6152	11.139633	-0.0022381	6.55E-07	-7.61E-11	3.33E-15	25024.974	-43.051299	34193.019
NO2-										
0	-12820.69477	699.01401	-2.8125971	0.0241289	-2.83E-05	1.67E-08	-3.98E-12	-28099.157	40.635382	-200035.59
1	132570.5145	-1557.0309	8.1267208	-2.73E-04	-4.71E-08	2.83E-11	-2.35E-15	-17157.96	-22.28309	-200035.59
NO2CL										
0	8508.37034	-180.53838	3.7853886	0.0141493	-1.42E-05	7.03E-09	-1.37E-12	915.62465	6.9588997	12500
1	-108677.3327	-1452.2312	11.05657	-4.00E-04	9.10E-08	-1.04E-11	4.78E-16	6294.2673	-35.212402	12500
NO2F										
0	56678.5695	-653.8252	4.4727715	0.0136887	-1.46E-05	7.78E-09	-1.69E-12	-11021.794	0.3292084	-109000
1	-100857.7842	-1704.7228	11.229549	-4.69E-04	1.05E-07	-1.19E-11	5.47E-16	-6891.7192	-38.497884	-109000
NO3										
0	34053.9841	226.66707	-3.7930816	0.0417073	-5.71E-05	3.83E-08	-1.02E-11	7088.1122	42.730918	71128
1	-394387.271	-824.42635	10.613258	-2.45E-04	5.41E-08	-6.20E-12	2.87E-16	8982.0117	-34.446665	71128
NO3-										
0	92048.1361	-391.11712	-0.2354357	0.0283604	-3.46E-05	2.08E-08	-5.02E-12	-35764.115	22.999424	-310779.53
1	-311000.5758	-1369.0876	11.013429	-4.04E-04	8.90E-08	-1.02E-11	4.72E-16	-33643.211	-38.784326	-310779.53
NO3F										
0	64728.9486	-821.32149	6.1949554	0.0180543	-2.00E-05	1.12E-08	-2.68E-12	4206.7015	-7.0163224	15000
1	-341211.507	-2353.8235	16.281063	-0.0019104	4.69E-07	-5.69E-11	2.72E-15	9760.031	-65.580909	15000
N2										
0	22103.71497	-381.84618	6.0827384	-0.0085309	1.38E-05	-9.63E-09	2.52E-12	710.84609	-10.760033	0
1	587712.406	-2239.2491	6.0669492	-6.14E-04	1.49E-07	-1.92E-11	1.06E-15	12832.104	-15.866396	0
2	8.31E+08	-642073.35	202.02646	-0.0306509	2.49E-06	-9.71E-11	1.44E-15	4938707	-1672.0997	0
N2+										
0	-34740.4747	269.62227	3.1649164	-0.0021322	6.73E-06	-5.64E-09	1.62E-12	179000.44	6.8329784	1509508.4
1	-2845599.002	7058.893	-2.8848864	0.0030687	-4.36E-07	2.10E-11	5.41E-16	134038.85	50.908974	1509508.4
2	-3.71E+08	313928.72	-96.035181	0.0157119	-1.18E-06	4.14E-11	-5.62E-16	-2217361.9	843.6271	1509508.4
N2-										

0	0	0	3.8826848	-0.0031924	8.52E-06	-7.34E-09	2.21E-12	16796.935	3.1118052	148617.44
1	0	0	3.1156753	0.0014589	-6.02E-07	1.13E-10	-7.97E-15	16859.058	6.389856	148617.44
NCN										
0	-74464.8956	965.73425	-1.4640866	0.0194656	-2.05E-05	1.08E-08	-2.30E-12	54211.379	33.581669	500795.49
1	-148726.101	-774.54901	7.995153	-1.63E-04	2.89E-08	-3.02E-12	1.98E-16	61923.385	-21.130863	500795.49
cis-N2D2										
0	-27436.7252	714.97227	-2.2232011	0.0208871	-1.82E-05	8.84E-09	-1.92E-12	20622.433	36.370745	207108
1	879816.913	-5299.3952	13.550117	-0.0013167	2.76E-07	-3.04E-11	1.37E-15	54074.561	-62.712451	207108
N2F2										
0	15438.9315	-218.36351	3.8902843	0.0167402	-2.06E-05	1.26E-08	-3.11E-12	7052.0387	5.2658683	62373.546
1	-182488.386	-953.403	10.697955	-2.76E-04	6.06E-08	-6.91E-12	3.19E-16	9283.467	-32.469686	62373.546
N2F4										
0	116289.688	-1538.6386	9.0539346	0.0286213	-4.33E-05	3.07E-08	-8.46E-12	2865.1692	-24.764357	-22000
1	-518807.373	-670.39791	16.501309	-2.01E-04	4.44E-08	-5.10E-12	2.36E-16	-5280.4097	-60.406659	-22000
N2H2										
0	-150400.5163	2346.6877	-9.4054303	0.032843	-3.12E-05	1.72E-08	-4.01E-12	13193.84	78.32383	211858.76
1	6217567.87	-17539.521	20.227305	-9.76E-04	-4.21E-07	1.12E-10	-7.63E-15	137415.26	-119.95591	211858.76
NH2NO2										
0	-45730.3506	1201.366	-8.1059841	0.0540272	-6.44E-05	4.03E-08	-1.03E-11	-9615.7852	68.673536	-26000
1	1654040.575	-8125.2209	20.217428	-0.0012443	2.12E-07	-1.95E-11	7.44E-16	42308.226	-101.61902	-26000
N2H4										
0	-166075.6354	3035.4167	-17.368898	0.0715983	-8.87E-05	5.80E-08	-1.53E-11	-3731.9272	119.00023	95180
1	3293486.7	-11998.506	21.044068	-0.0013994	1.93E-07	-1.32E-11	3.17E-16	83484.337	-115.5751	95180
N2O										
0	42882.2597	-644.01184	6.0343514	2.27E-04	3.47E-06	-3.63E-09	1.14E-12	11794.055	-10.031283	81600
1	343844.804	-2404.5576	9.1256362	-5.40E-04	1.32E-07	-1.41E-11	6.38E-16	21986.326	-31.478047	81600
N2O+										
0	-56286.1325	670.12104	0.0855799	0.0152499	-1.53E-05	7.83E-09	-1.65E-12	155732.24	25.636431	1333000
1	-29899.5589	-1179.2895	8.3000231	-2.89E-04	5.70E-08	-5.96E-12	2.83E-16	164606.32	-22.872368	1333000
N2O3										
0	-92044.4417	929.55202	3.2036648	0.0135647	-6.26E-06	-1.40E-09	1.43E-12	3313.6221	18.444311	86630.595
1	778388.186	-4483.0247	16.66668	-0.0020621	5.31E-07	-6.19E-11	2.69E-15	33609.125	-67.392122	86630.595
N2O4										
0	-38047.5144	561.28289	-0.2083648	0.0388709	-4.42E-05	2.50E-08	-5.68E-12	-3310.7947	29.63925	11110.919
1	-458284.376	-1604.7498	16.741021	-5.09E-04	1.14E-07	-1.32E-11	5.98E-16	4306.9005	-65.694503	11110.919
N2O5										
0	40078.2817	-876.96751	10.55933	0.0139461	-8.88E-06	8.50E-10	7.79E-13	3038.962	-23.868317	13300
1	-53255.7896	-3109.2774	20.36089	-9.96E-04	2.40E-07	-3.06E-11	1.50E-15	13369.573	-82.986232	13300
N3										
0	33374.0679	-296.56836	3.3142792	0.0067217	-4.18E-06	8.62E-10	6.88E-14	52988.406	5.3127808	436000
1	252926.4658	-2362.8766	9.1352671	-6.21E-04	1.32E-07	-1.48E-11	6.72E-16	64126.954	-31.358255	436000
N3H										
0	3242.57606	66.926649	1.7661422	0.0148741	-1.54E-05	9.17E-09	-2.34E-12	33920.697	15.137525	294000
1	1170469.241	-5102.452	12.782889	-8.41E-04	1.59E-07	-1.51E-11	6.10E-16	64283.445	-55.131187	294000
Na										
0	0	0	2.5	0	0	0	0	12183.829	4.2440282	107500
1	952572.338	-2623.8073	5.1625966	-0.0012102	2.31E-07	-1.25E-11	7.23E-16	29129.636	-15.197171	107500
2	1.59E+09	-971783.67	223.8444	-0.0238093	1.35E-06	-3.94E-11	4.63E-16	7748677.3	-1939.6155	107500
Na+										
0	0	0	2.5	0	0	0	0	72565.371	3.5508452	609542.93
1	0	0	2.5	0	0	0	0	72565.371	3.5508452	609542.93
2	34012.0299	-21.377746	2.5054439	-7.19E-07	5.19E-11	-1.94E-15	2.96E-20	72734.136	3.5039042	609542.93
Na-										
0	0	0	2.5	0	0	0	0	5082.1997	3.5509168	48453.428
1	0	0	2.5	0	0	0	0	5082.1997	3.5509168	48453.428
2	0	0	2.5	0	0	0	0	5082.1997	3.5509168	48453.428
NaALF4										
0	0	0	4.3052145	0.044968	-7.43E-05	5.81E-08	-1.75E-11	-224149.88	6.371846	-1840979.9
1	0	0	14.271553	0.00198	-8.82E-07	1.73E-10	-1.25E-14	-226123.47	-41.275518	-1840979.9
NaBO2										
0	0	0	4.0654749	0.0134549	-1.39E-05	6.64E-09	-1.07E-12	-79700.157	7.9348163	-648530.98
1	0	0	7.496525	0.002631	-1.10E-06	2.05E-10	-1.42E-14	-80578.591	-9.4463018	-648530.98
NaBr										
0	0	0	3.901089	0.0025025	-3.89E-06	2.83E-09	-7.72E-13	-18556.161	6.1887933	-143931.77
1	0	0	4.4433135	1.58E-04	-2.80E-08	5.38E-12	-3.81E-16	-18659.489	3.6085822	-143931.77
NaCN										
0	0	0	4.9772558	0.0053226	-7.56E-06	6.18E-09	-2.01E-12	9673.149	-0.3882256	94271.689
1	0	0	5.7989775	0.0016828	-6.74E-07	1.22E-10	-8.30E-15	9493.3444	-4.3442787	94271.689
NaCL										
0	0	0	3.7032286	0.0031998	-4.89E-06	3.46E-09	-9.14E-13	-23028.276	5.7734795	-181412.21
1	0	0	4.4282931	1.56E-04	-2.81E-08	4.72E-12	-2.88E-16	-23170.9	2.3009746	-181412.21
NaF										
0	0	0	2.7487183	0.0080324	-1.52E-05	1.34E-08	-4.45E-12	-36000.207	8.6810782	-290453
1	0	0	4.333768	2.57E-04	-6.94E-08	1.20E-11	-7.49E-16	-36279.787	1.3004636	-290453
NaF2-										
0	0	0	4.5826889	0.0106052	-1.57E-05	1.06E-08	-2.64E-12	-82234.497	1.4892077	-669451.53
1	0	0	7.1223193	4.19E-04	-1.80E-07	3.40E-11	-2.38E-15	-82755.73	-10.786674	-669451.53
NaH										
0	0	0	3.120395	0.0013996	2.21E-06	-4.00E-09	1.67E-12	13940.065	4.3945613	124260.98
1	0	0	3.8130579	8.56E-04	-3.12E-07	5.85E-11	-4.05E-15	13683.062	0.4841682	124260.98
NaI										
0	0	0	4.0406275	0.0019687	-3.05E-06	2.26E-09	-6.23E-13	-11988.041	6.4598011	-89120.307

1	0	0	4.458457	1.42E-04	-1.69E-08	3.90E-12	-2.80E-16	-12066.843	4.4759588	-89120.307
NaO										
0	0	0	3.4421007	0.0041617	-6.31E-06	4.45E-09	-1.17E-12	8901.1477	6.9503254	83684.358
1	0	0	4.3924158	2.13E-04	-4.52E-08	7.98E-12	-5.17E-16	8711.8995	2.3880897	83684.358
NaO-										
0	0	0	3.4186855	0.0042117	-6.31E-06	4.39E-09	-1.14E-12	-15752.234	5.6685565	-121336.75
1	0	0	4.3868008	2.23E-04	-4.82E-08	8.57E-12	-5.61E-16	-15946.268	1.0136349	-121336.75
NaOH										
0	34420.0907	-792.31841	8.9979172	-0.0040798	3.07E-06	-5.12E-10	-1.54E-13	-20869.528	-25.105813	-191000
1	875381.549	-2342.5216	7.9784764	1.02E-04	-6.27E-08	1.02E-11	-5.71E-16	-9509.8565	-22.023152	-191000
NaOH+										
0	0	0	4.3505204	0.0087465	-1.46E-05	1.14E-08	-3.21E-12	79946.399	2.3448408	677830.54
1	0	0	5.6688547	0.0012254	-3.40E-07	4.29E-11	-1.96E-15	79806.514	-3.4246826	677830.54
Na2										
0	0	0	4.1156826	0.002529	-5.62E-06	6.46E-09	-2.75E-12	15782.462	3.6867245	142043.13
1	0	0	5.962019	-0.0010605	-4.39E-07	3.05E-10	-3.39E-14	14999.093	-6.6961363	142043.13
Na2C2N2										
0	0	0	10.368029	0.0133485	-1.99E-05	1.62E-08	-5.13E-12	-4593.7527	-20.549461	-8776.984
1	0	0	12.572786	0.0033947	-1.36E-06	2.47E-10	-1.68E-14	-5049.1021	-31.074216	-8776.984
Na2CL2										
0	0	0	7.9583953	0.0083962	-1.38E-05	1.03E-08	-2.86E-12	-70725.939	-8.1753247	-566077.38
1	0	0	9.8262001	1.92E-04	-8.16E-08	1.53E-11	-1.06E-15	-71077.149	-17.036101	-566077.38
Na2F2										
0	0	0	4.8212191	0.0198364	-3.06E-05	2.13E-08	-5.53E-12	-103890.05	2.3662548	-846432.82
1	0	0	9.433553	6.36E-04	-2.76E-07	5.29E-11	-3.73E-15	-104801.14	-19.752992	-846432.82
Na2O										
0	0	0	4.7787177	0.0099488	-1.48E-05	1.00E-08	-2.51E-12	-6736.0206	1.7994763	-41417.546
1	0	0	7.1470582	3.98E-04	-1.74E-07	3.36E-11	-2.38E-15	-7219.1261	-9.6348105	-41417.546
Na2O2H2										
0	108941.9856	-2634.8312	23.066138	-0.0168932	1.67E-05	-7.82E-09	1.48E-12	-65931.333	-98.030147	-624000
1	1675692.516	-4704.8673	16.973387	1.96E-04	-1.24E-07	2.03E-11	-1.13E-15	-48562.808	-68.134429	-624000
Na2SO4										
0	0	0	2.0727498	0.054582	-7.85E-05	5.51E-08	-1.53E-11	-126769.55	16.668826	-1033641.6
1	0	0	15.206128	0.0042984	-1.90E-06	3.72E-10	-2.68E-14	-129673.57	-47.656922	-1033641.6
Nb										
0	78896.6067	-1212.8139	10.345798	-0.0167663	1.98E-05	-1.22E-08	3.06E-12	91653.151	-35.947429	723113.1
1	-1096553.196	2546.6507	2.2360549	-0.00128	8.46E-07	-1.49E-10	8.71E-15	68791.246	13.98169	723113.1
2	1.82E+09	-1032414.9	230.8238	-0.02445	1.40E-06	-4.09E-11	4.83E-16	8359622.6	-1997.7973	723113.1
Nb+										
0	131444.7859	-2000.135	15.050242	-0.0299658	3.73E-05	-2.27E-08	5.45E-12	176005.4	-62.245955	1393604.7
1	-1077639.646	2159.0464	2.3106048	-5.36E-04	5.06E-07	-1.03E-10	6.63E-15	151794.55	12.106785	1393604.7
2	1.88E+07	-22028.479	14.270045	-0.0022959	2.43E-07	-1.12E-11	1.84E-16	324541.56	-84.945557	1393604.7
Nb-										
0	-72209.2485	525.95013	3.4704684	-0.0049505	7.40E-06	-5.02E-09	1.31E-12	71788.289	5.1555101	631054.01
1	111745.8019	134.00728	2.3914741	4.52E-05	-1.03E-08	1.20E-12	-5.61E-17	74739.968	9.6753156	631054.01
2	-127944.668	166.42651	2.4633343	4.16E-06	-2.57E-10	8.24E-15	-1.07E-19	74304.339	9.1861885	631054.01
NbCL5										
0	73482.7797	-1919.173	22.907996	-0.0140435	1.64E-05	-1.02E-08	2.61E-12	-79741.188	-84.396379	-703330
1	-156381.6638	-44.505213	16.035446	-1.49E-05	3.42E-09	-4.04E-13	1.92E-17	-89628.151	-43.745834	-703330
NbO										
0	0	0	2.9214485	0.0031324	-1.49E-06	-9.93E-10	8.00E-13	22907.886	11.236294	198744.99
1	0	0	3.8811729	8.20E-04	-4.25E-07	1.03E-10	-8.04E-15	22637.132	6.2236415	198744.99
NbOCL3										
0	-110848.2359	117.3067	11.655584	0.0012874	-1.66E-06	1.10E-09	-2.95E-13	-95040.239	-23.864507	-752300
1	-151555.1427	53.055452	12.289153	-1.53E-04	6.78E-08	-9.37E-12	4.67E-16	-94907.681	-27.452645	-752300
NbO2										
0	0	0	3.5767268	0.006359	-5.96E-07	-6.34E-09	3.71E-12	-25387.319	10.625701	-200000
1	0	0	6.0514795	9.75E-04	-3.83E-07	6.54E-11	-4.07E-15	-26100.865	-2.4001566	-200000
Ne										
0	0	0	2.5	0	0	0	0	-745.375	3.3553227	0
1	0	0	2.5	0	0	0	0	-745.375	3.3553227	0
2	-1.24E+07	6958.5796	1.0167093	1.42E-04	-4.80E-09	-1.17E-13	8.42E-18	-56639.336	16.484387	0
Ne+										
0	72815.5148	-869.5698	6.108647	-0.0058414	5.04E-06	-2.29E-09	4.34E-13	254599.69	-16.734494	2086965.9
1	-111274.2634	476.56979	2.1966505	1.10E-04	-2.29E-08	2.51E-12	-1.13E-16	247253.69	7.4661405	2086965.9
2	-56150.9457	141.89588	2.4757173	1.94E-06	-6.32E-11	-1.31E-16	3.53E-20	249445.24	5.366878	2086965.9
Ni										
0	-32358.1055	601.52646	-1.0792707	0.0108951	-1.37E-05	8.32E-09	-2.02E-12	48138.108	27.188292	430116.61
1	-493826.221	1092.91	2.410485	-1.60E-05	-1.05E-08	4.62E-12	-4.45E-17	43360.722	9.6771956	430116.61
2	3.49E+08	-165422.76	33.498694	-0.0035271	3.24E-07	-1.60E-11	2.94E-16	1409017.8	-267.24556	430116.61
Ni+										
0	-89693.8603	1173.6015	-3.4106204	0.0139074	-1.50E-05	7.90E-09	-1.65E-12	134558.95	40.314952	1172594.6
1	-3961999.32	10170.849	-6.0293313	0.0027709	-8.90E-08	-5.54E-11	5.24E-15	73403.951	71.375031	1172594.6
2	5.29E+07	-37198.271	14.707944	-0.0014893	8.65E-08	-1.71E-12	5.05E-18	425320.41	-95.905022	1172594.6
Ni-										
0	-84376.2475	1135.4766	-3.3806158	0.01423	-1.58E-05	8.61E-09	-1.88E-12	31243.076	39.980613	311764.36
1	-543342.48	1182.6453	2.1264412	3.73E-05	6.95E-09	-1.95E-12	1.27E-16	28547.591	10.434622	311764.36
2	2235741.343	-753.93211	2.675777	-2.06E-05	1.30E-09	-4.21E-14	5.52E-19	43591.144	5.7245166	311764.36
NiCL										
0	0	0	3.4897757	0.0031838	-1.91E-06	-3.57E-10	4.61E-13	20725.935	9.5497444	182008.9
1	0	0	5.5836514	-0.001433	8.52E-07	-1.49E-10	8.16E-15	20056.505	-1.6373214	182008.9
NiCL2										

0	0	0	4.5606177	0.0136137	-2.37E-05	1.96E-08	-6.24E-12	-10683.571	6.2361942	-73932.233
1	0	0	7.387453	8.46E-04	-4.31E-07	9.36E-11	-7.19E-15	-11235.857	-7.188951	-73932.233
NiO										
0	0	0	2.9919682	0.0033309	-1.54E-06	-1.56E-09	1.21E-12	36742.094	9.8214074	314003.74
1	0	0	4.1046114	4.87E-04	-1.88E-07	3.55E-11	-2.47E-15	36445.645	4.0767966	314003.74
NiS										
0	0	0	3.1168107	0.0040174	-1.56E-06	-1.51E-09	9.37E-13	41896.857	11.467735	357427.4
1	0	0	4.9160472	3.14E-04	-2.97E-07	8.02E-11	-6.73E-15	41321.032	1.818988	357427.4
O										
0	-7953.6113	160.71778	1.9662264	0.0010137	-1.11E-06	6.52E-10	-1.58E-13	28403.624	8.4042418	249175
1	261902.0262	-729.8722	3.3171773	-4.28E-04	1.04E-07	-9.44E-12	2.73E-16	33924.281	-0.6679585	249175
2	1.78E+08	-108232.83	28.107784	-0.0029752	1.85E-07	-5.80E-12	7.19E-17	889094.26	-218.17282	249175
O+										
0	0	0	2.5	0	0	0	0	187935.28	4.3933768	1568787.2
1	-216651.3208	666.54562	1.7020644	4.71E-04	-1.43E-07	2.02E-11	-9.11E-16	183719.2	10.056904	1568787.2
2	-2.14E+08	146951.85	-36.808645	0.0050362	-3.09E-07	9.19E-12	-1.07E-16	-961420.9	342.61931	1568787.2
O-										
0	-5695.85711	109.92873	2.1847197	5.33E-04	-5.30E-07	2.87E-10	-6.52E-14	10932.875	6.7298639	101846.19
1	9769.36318	7.1596048	2.4949617	1.97E-06	-4.30E-10	4.91E-14	-2.27E-18	11495.544	4.8370364	101846.19
2	566.2391	7.5723403	2.4983525	1.86E-07	-1.15E-11	3.69E-16	-4.79E-21	11484.26	4.8134066	101846.19
OD										
0	21186.91536	-278.59824	5.4562101	-0.0061481	9.12E-06	-5.53E-09	1.24E-12	4711.375	-7.6166189	37221.508
1	783247.316	-2532.9926	5.9521247	-3.74E-04	4.96E-08	3.45E-12	-7.38E-16	19551.427	-15.688984	37221.508
OD-										
0	56061.2832	-751.41562	7.5441885	-0.0109208	1.50E-05	-9.35E-09	2.25E-12	-14895.483	-21.064984	-145382.9
1	302946.7029	-1079.6847	4.2114174	6.26E-04	-2.41E-07	4.25E-11	-2.39E-15	-11627.763	-4.7248988	-145382.9
OH										
0	-1998.85899	93.001362	3.0508542	0.0015295	-3.16E-06	3.32E-09	-1.14E-12	3239.6835	4.6741108	39344.106
1	1017393.379	-2509.9573	5.1165479	1.31E-04	-8.28E-08	2.01E-11	-1.56E-15	20444.871	-11.012823	39344.106
2	2.85E+08	-185953.26	50.082409	-0.0051424	2.88E-07	-8.23E-12	9.57E-17	1468642.4	-402.35556	39344.106
OH+										
0	60316.3086	-757.35203	7.3077529	-0.0095069	1.20E-05	-6.83E-09	1.50E-12	157858	-19.50107	1290331.5
1	504072.91	-1380.053	4.1254622	8.33E-04	-3.44E-07	6.79E-11	-4.36E-15	163315.71	-3.9970585	1290331.5
2	1.16E+09	-684128.04	157.61946	-0.0161842	8.85E-07	-2.48E-11	2.81E-16	5615529	-1351.879	1290331.5
OH-										
0	29108.80827	-321.69049	4.8510291	-0.002579	2.00E-06	-7.96E-11	-2.32E-13	-16640.393	-7.1215913	-143190.3
1	471133.117	-857.23367	3.1661812	0.0012336	-4.00E-07	6.24E-11	-3.35E-15	-12000.022	1.4877363	-143190.3
O2										
0	-34255.6342	484.7001	1.119011	0.0042939	-6.84E-07	-2.02E-09	1.04E-12	-3391.4549	18.496995	0
1	-1037939.022	2344.8303	1.819732	0.0012678	-2.19E-07	2.05E-11	-8.19E-16	-16890.109	17.387165	0
2	4.98E+08	-286610.69	66.903523	-0.00617	3.02E-07	-7.42E-12	7.28E-17	2293554	-553.06216	0
O2+										
0	-86072.0545	1051.8759	-0.543238	0.0065712	-3.27E-06	5.94E-11	3.24E-13	134554.47	29.027098	1171828.4
1	73846.5488	-845.95595	4.9851642	-1.61E-04	6.43E-08	-1.50E-11	1.58E-15	144632.1	-5.8112307	1171828.4
2	-1.56E+09	1161406.8	-330.25047	0.0471094	-3.35E-06	1.17E-10	-1.59E-15	-8857866.3	2852.0356	1171828.4
O2-										
0	18839.445	114.94603	1.5189264	0.008016	-9.85E-06	6.04E-09	-1.49E-12	-7101.4944	15.011828	-48027.921
1	-56583.5514	-236.69398	4.6757392	-2.19E-05	1.71E-08	-1.76E-12	8.24E-17	-5960.741	-2.4362052	-48027.921
O3										
0	-12760.59932	589.00776	-2.543736	0.0268927	-3.53E-05	2.31E-08	-6.04E-12	13487.685	38.500429	141800
1	-2.76E+07	71528.207	-57.35735	0.0206731	2.07E-07	-8.53E-10	8.33E-14	-453216.2	469.24929	141800
P										
0	50.4086657	-0.7639419	2.504564	-1.38E-05	2.25E-08	-1.87E-11	6.23E-15	37324.219	5.3593035	316500
1	1261794.642	-4559.8382	8.9180793	-0.0043814	1.45E-06	-2.03E-10	1.02E-14	65417.24	-39.159748	316500
2	-2.22E+07	-45669.112	28.372454	-0.0044832	3.58E-07	-1.26E-11	1.59E-16	337090.58	-205.69609	316500
P+										
0	-73169.0811	962.79791	-0.3693938	0.0047668	-4.57E-06	2.37E-09	-5.13E-13	154940.68	23.766408	1336453.5
1	-559424.936	1722.5765	0.8430381	6.29E-04	-6.32E-08	-1.81E-12	4.32E-16	149049.34	18.452752	1336453.5
2	1.36E+07	-8717.5024	4.7474263	-1.62E-04	-3.94E-10	4.85E-13	-7.45E-18	228464.97	-13.464549	1336453.5
P-										
0	-10089.49093	182.64684	1.9624563	9.20E-04	-9.21E-07	5.01E-10	-1.14E-13	27030.824	9.4781378	238826.77
1	15434.88016	9.4950093	2.4931709	2.70E-06	-5.95E-10	6.82E-14	-3.17E-18	27975.727	6.2467939	238826.77
2	1724.147889	10.748325	2.4976549	2.66E-07	-1.64E-11	5.27E-16	-6.85E-21	27954.83	6.2158493	238826.77
PCL										
0	34888.617	-560.31193	6.2645685	-0.0031834	3.50E-06	-2.09E-09	5.42E-13	17746.538	-8.0745789	134615.11
1	-347168.151	993.55579	3.3994303	4.02E-04	8.30E-08	-3.09E-11	2.11E-15	8433.5912	10.649016	134615.11
PCL2										
0	51900.845	-1060.9042	10.585499	-0.0068799	7.62E-06	-4.53E-09	1.12E-12	-3220.3312	-27.535192	-54292.353
1	-83498.3397	-26.252495	7.0203618	-8.39E-06	1.90E-09	-2.21E-13	1.04E-17	-8742.9937	-6.234032	-54292.353
PCL2-										
0	49348.3277	-960.15905	9.8847697	-0.0049502	4.95E-06	-2.68E-09	6.08E-13	-39980.724	-24.131326	-356285.25
1	-85649.8676	-31.855559	7.024495	-1.00E-05	2.25E-09	-2.62E-13	1.23E-17	-45038.114	-6.7215312	-356285.25
PCL3										
0	77177.4547	-1617.6509	15.360805	-0.0101108	1.10E-05	-6.48E-09	1.58E-12	-29558.936	-52.443397	-289500
1	-133307.693	-41.458832	10.031861	-1.30E-05	2.92E-09	-3.39E-13	1.59E-17	-38003.367	-20.507387	-289500
PCL5										
0	102907.02	-2515.7075	24.30115	-0.0156461	1.71E-05	-1.01E-08	2.46E-12	-37225.824	-98.163363	-376000
1	-225590.689	-69.385428	16.053596	-2.20E-05	4.97E-09	-5.80E-13	2.73E-17	-50342.342	-48.72456	-376000
PF										
0	22278.66728	-172.75087	3.0853669	0.0054897	-8.25E-06	5.87E-09	-1.62E-12	-5809.2797	7.7097189	-47944.793
1	-1132572.282	3200.0386	0.7780502	0.0019695	-4.37E-07	5.24E-11	-2.62E-15	-27667.73	27.593123	-47944.793
PF+										

0	0	0	3.9402122	-5.38E-04	3.94E-06	-4.67E-09	1.74E-12	107252.6	4.5185033	901540.87
1	0	0	4.0816184	4.95E-04	-2.03E-07	3.92E-11	-2.78E-15	107145.85	3.4444167	901540.87
PF-										
0	0	0	3.5951376	0.0030313	-4.41E-06	3.16E-09	-8.92E-13	-20904.094	5.8699065	-164050.12
1	0	0	4.3037691	2.64E-04	-9.88E-08	1.87E-11	-1.21E-15	-21058.144	2.4122915	-164050.12
PFCL										
0	54901.8853	-865.86795	7.9444677	9.50E-04	-3.34E-06	3.02E-09	-9.45E-13	-31328.432	-14.404274	-283184.12
1	-128214.3211	-97.390436	7.0726617	-2.90E-05	6.41E-09	-7.34E-13	3.40E-17	-36006.493	-7.6264983	-283184.12
PFCL-										
0	89343.3685	-1266.9725	9.9121945	-0.0038779	3.04E-06	-1.30E-09	2.32E-13	-58945.057	-26.17051	-529269.11
1	-123156.515	-97.658611	7.0740296	-3.00E-05	6.69E-09	-7.72E-13	3.60E-17	-65588.172	-8.2088833	-529269.11
PFCL2										
0	82665.6056	-1512.1389	13.034042	-0.0029032	7.84E-07	6.46E-10	-3.74E-13	-56442.379	-41.009064	-511925.34
1	-186458.9813	-114.80044	10.085998	-3.45E-05	7.63E-09	-8.75E-13	4.06E-17	-64504.722	-21.740553	-511925.34
PFCL-										
0	89343.3685	-1266.9725	9.9121945	-0.0038779	3.04E-06	-1.30E-09	2.32E-13	-58945.057	-26.17051	-529269.11
1	-123156.515	-97.658611	7.0740296	-3.00E-05	6.69E-09	-7.72E-13	3.60E-17	-65588.172	-8.2088833	-529269.11
PFCL4										
0	141207.1573	-2882.4711	23.873452	-0.0123951	1.14E-05	-5.71E-09	1.20E-12	-66134.787	-98.596945	-635016.44
1	-295437.588	-132.51543	16.100054	-4.04E-05	8.97E-09	-1.03E-12	4.80E-17	-81357.194	-50.624049	-635016.44
PF2										
0	55247.6572	-628.05178	5.1374379	0.0091207	-1.47E-05	1.08E-08	-3.06E-12	-59775.415	-1.6895895	-513103.66
1	-170846.712	-169.20515	7.1254916	-4.99E-05	1.10E-08	-1.25E-12	5.78E-17	-63382.958	-10.417157	-513103.66
PF2-										
0	140479.3057	-1699.9458	10.36824	-0.0035996	1.96E-06	-3.83E-10	-3.38E-14	-78104.345	-32.173752	-709337.95
1	-165397.6056	-164.06048	7.1240915	-5.02E-05	1.12E-08	-1.29E-12	6.00E-17	-87002.233	-11.090749	-709337.95
PF2CL										
0	83975.9016	-1318.0759	10.172035	0.0055712	-1.10E-05	8.73E-09	-2.57E-12	-83816.562	-27.660134	-735076.68
1	-240928.1185	-203.34847	10.151508	-6.05E-05	1.33E-08	-1.53E-12	7.06E-17	-91011.106	-24.17826	-735076.68
PF2CL3										
0	184209.9543	-3334.4024	23.885109	-0.0103094	7.36E-06	-2.50E-09	2.51E-13	-92795.499	-102.79916	-878744.96
1	-365527.254	-202.96942	16.15238	-6.12E-05	1.36E-08	-1.56E-12	7.22E-17	-110494.15	-53.87309	-878744.96
PF3										
0	84806.3579	-1102.2934	7.1604696	0.0143834	-2.32E-05	1.70E-08	-4.81E-12	-111183.98	-14.57514	-957400
1	-295719.008	-299.7176	10.222904	-8.89E-05	1.96E-08	-2.24E-12	1.03E-16	-117374.67	-27.773725	-957400
PF3CL2										
0	182249.7206	-3089.6102	20.677104	-0.0011687	-5.02E-06	5.80E-09	-1.97E-12	-122812.07	-86.279779	-1122022.9
1	-422383.805	-320.79652	16.24013	-9.62E-05	2.13E-08	-2.44E-12	1.13E-16	-139264.22	-55.312863	-1122022.9
PF4CL										
0	180424.0323	-2741.0966	16.801928	0.0099193	-2.03E-05	1.62E-08	-4.77E-12	-153238.26	-66.791203	-1364909.4
1	-478114.004	-426.48128	16.318121	-1.27E-04	2.81E-08	-3.22E-12	1.49E-16	-168048.84	-57.358451	-1364909.4
PF5										
0	185572.549	-2436.9118	12.009798	0.0233942	-3.81E-05	2.80E-08	-7.87E-12	-181456.99	-44.863017	-1593300
1	-566945.952	-667.56959	16.497633	-1.99E-04	4.39E-08	-5.03E-12	2.33E-16	-194433.57	-62.615342	-1593300
PH										
0	22736.33198	-397.26741	6.2336977	-0.0091818	1.52E-05	-1.09E-08	2.93E-12	28527.684	-10.951912	230752.1
1	781473.065	-3038.4512	7.467481	-0.0018375	7.17E-07	-1.14E-10	6.18E-15	45362.602	-24.672981	230752.1
PH2										
0	15553.1601	-184.1675	4.8959395	-0.0034956	1.05E-05	-8.38E-09	2.27E-12	14098.429	-2.2108036	119553.47
1	1127878.16	-4715.2201	10.214964	-0.0011676	2.15E-07	-1.62E-11	3.77E-16	41830.629	-42.316096	119553.47
PH2-										
0	69506.8449	-771.91629	7.3835376	-0.0085229	1.47E-05	-9.85E-09	2.41E-12	1582.2959	-17.613064	-9265.418
1	1382525.815	-5213.4007	10.216948	-0.0011163	2.22E-07	-2.34E-11	1.02E-15	29906.837	-43.787116	-9265.418
PH3										
0	0	0	3.1581935	0.0024941	9.03E-06	-1.02E-08	3.28E-12	-461.23725	6.2372248	5423.662
1	0	0	3.3448794	0.0065771	-2.63E-06	4.77E-10	-3.24E-14	-816.17675	3.9547962	5423.662
PN										
0	-51032.0384	820.29267	-1.3927728	0.0128799	-1.40E-05	7.78E-09	-1.75E-12	15732.265	32.510708	171487.31
1	-249562.5593	176.04388	4.144122	2.48E-04	-5.67E-08	4.26E-12	3.06E-16	17703.173	1.3255187	171487.31
PO										
0	-68457.5406	1141.2957	-2.7795561	0.0167846	-1.97E-05	1.19E-08	-2.93E-12	-9847.745	41.843283	-27857.687
1	-336666.744	622.93558	3.5656055	6.52E-04	-2.06E-07	3.18E-11	-1.57E-15	-8939.7904	6.9548592	-27857.687
PO-										
0	54343.4632	-412.36236	3.7464839	0.0038586	-5.96E-06	4.28E-09	-1.14E-12	-15558.109	3.4044365	-140067.09
1	-848.029478	347.05449	2.8778902	0.0016222	-4.87E-07	6.65E-11	-3.40E-15	-19872.095	10.754444	-140067.09
POCL3										
0	47937.8816	-1270.3883	13.677165	0.0010827	-1.74E-06	8.46E-10	-1.17E-13	-65075.719	-43.147068	-568400
1	-218593.797	-508.02697	13.377847	-1.51E-04	3.34E-08	-3.84E-12	1.78E-16	-70093.151	-39.847472	-568400
POFCL2										
0	46940.6156	-1069.2426	10.712843	0.0094912	-1.31E-05	8.43E-09	-2.14E-12	-92748.95	-28.150784	-793889.31
1	-270764.7503	-655.65023	13.486684	-1.94E-04	4.29E-08	-4.92E-12	2.28E-16	-96543.921	-41.649642	-793889.31
POF2CL										
0	52264.3816	-969.10377	7.963636	0.017556	-2.40E-05	1.57E-08	-4.08E-12	-120265.69	-15.939674	-1022607
1	-334708.659	-817.61048	13.606643	-2.42E-04	5.34E-08	-6.13E-12	2.84E-16	-123340.12	-44.961038	-1022607
POF3										
0	29660.3071	-427.67058	3.6691461	0.0283949	-3.77E-05	2.45E-08	-6.34E-12	-150112.45	5.160418	-1252000
1	-369060.242	-1005.5525	13.745299	-2.97E-04	6.55E-08	-7.51E-12	3.48E-16	-149976.17	-48.822142	-1252000
PO2										
0	-63726.6499	1036.7363	-2.8777722	0.0227813	-2.57E-05	1.47E-08	-3.39E-12	-39935.425	44.25295	-281527.24
1	492601.32	-2605.4147	9.5175541	-0.0011803	2.53E-07	-1.79E-11	1.80E-16	-20289.179	-29.697058	-281527.24
PO2-										
0	27024.40495	29.397586	1.1626951	0.015999	-1.98E-05	1.21E-08	-2.96E-12	-72859.453	19.63113	-597623.75

1	1628679.172	-5989.1999	13.693188	-0.0036238	9.49E-07	-1.04E-10	4.02E-15	-36859.596	-59.567961	-597623.75
PS										
0	-768.97868	-46.378241	4.1046492	0.0015553	-2.32E-06	1.66E-09	-4.63E-13	17078.758	4.230676	150431.32
1	-270272.9081	888.35482	3.1691901	0.0010225	-3.80E-07	7.02E-11	-4.27E-15	11215.105	11.473364	150431.32
P2										
0	30539.2251	-324.61776	4.0224638	0.0032321	-5.51E-06	4.20E-09	-1.22E-12	17969.109	1.6453503	144000
1	-780693.649	2307.9109	1.4117431	0.0021082	-7.36E-07	1.26E-10	-7.08E-15	1329.8247	21.697414	144000
P2O3										
0	-66457.5389	758.09006	0.9888437	0.0285988	-3.23E-05	1.83E-08	-4.21E-12	-88200.367	26.899145	-684645.27
1	-217534.411	-1369.902	14.01143	-4.02E-04	8.87E-08	-1.02E-11	4.70E-16	-79227.57	-47.394872	-684645.27
P2O4										
0	-43760.9126	490.51028	0.9643649	0.0388607	-4.68E-05	2.81E-08	-6.82E-12	-116899.78	23.795828	-933754.63
1	-367011.486	-1638.4237	17.211886	-4.83E-04	1.06E-07	-1.22E-11	5.65E-16	-109043.59	-67.142766	-933754.63
P2O5										
0	-29991.5922	-45.945066	6.9874868	0.028833	-3.10E-05	1.64E-08	-3.47E-12	-138190.14	-3.4005727	-1124370.4
1	-324708.016	-2016.9751	20.486993	-5.91E-04	1.30E-07	-1.49E-11	6.90E-16	-130629.02	-80.31643	-1124370.4
P3										
0	46933.5895	-864.35893	8.7342475	1.09E-05	-2.00E-06	2.10E-09	-6.92E-13	27748.473	-20.635873	210000
1	-125351.306	-83.067346	7.5619568	-2.47E-05	5.46E-09	-6.24E-13	2.89E-17	23087.223	-12.283106	210000
P3O6										
0	201449.3813	-3053.4881	16.021141	0.0431689	-6.38E-05	4.42E-08	-1.20E-11	-177650.38	-65.562679	-1575681
1	-878796.81	-1651.9881	27.722584	-4.86E-04	1.07E-07	-1.22E-11	5.61E-16	-190916.55	-122.06653	-1575681
P4										
0	120514.185	-2345.7118	17.739466	-0.0145631	1.59E-05	-9.31E-09	2.27E-12	16088.465	-70.885906	58900
1	-185870.586	-62.845469	10.048449	-1.99E-05	4.48E-09	-5.23E-13	2.46E-17	3848.2109	-24.772978	58900
P4O6										
0	376089.475	-5685.8326	29.142255	0.0225153	-4.51E-05	3.59E-08	-1.06E-11	-168856.25	-145.13599	-1606000
1	-1008997.24	-887.2754	28.660648	-2.64E-04	5.81E-08	-6.65E-12	3.07E-16	-199713.89	-128.18538	-1606000
P4O7										
0	321858.696	-4871.4447	24.544171	0.0401551	-6.52E-05	4.76E-08	-1.33E-11	-218451.74	-118.15048	-1984448
1	-1102947.375	-1511.0771	32.109795	-4.37E-04	9.52E-08	-1.08E-11	4.91E-16	-242909.65	-147.31409	-1984448
P4O8										
0	271932.6942	-4118.6004	20.287142	0.0568542	-8.40E-05	5.82E-08	-1.58E-11	-260453.97	-94.071621	-2302214.1
1	-1173177.311	-2200.633	35.630101	-6.49E-04	1.43E-07	-1.64E-11	7.57E-16	-278384.31	-167.9637	-2302214.1
P4O9										
0	219991.6395	-3336.4649	15.864131	0.0740245	-1.03E-04	6.94E-08	-1.84E-11	-301874.27	-69.979677	-2613979.1
1	-1233696.783	-2917.0328	39.177571	-8.74E-04	1.94E-07	-2.23E-11	1.04E-15	-312963.75	-189.71764	-2613979.1
P4O10										
0	167014.2268	-2540.2433	11.368534	0.0913781	-1.23E-04	8.08E-08	-2.11E-11	-341015.19	-46.434313	-2906223.4
1	-1337201.132	-3516.3823	42.604033	-0.0010374	2.29E-07	-2.62E-11	1.21E-15	-345951.51	-211.54989	-2906223.4
Pb										
0	1213.382285	-19.06116	2.6192995	-3.83E-04	6.69E-07	-6.06E-10	2.24E-13	22820.962	6.2013692	195200
1	-9084313.07	26726.732	-26.26244	0.0135828	-2.69E-06	2.35E-10	-7.32E-15	-148165.07	215.40116	195200
2	5.33E+08	-275141.92	63.030319	-0.0068137	4.45E-07	-1.52E-11	2.04E-16	2243651.7	-522.56499	195200
Pb+										
0	9.48668904	-0.1134956	2.5005498	-1.38E-06	1.91E-09	-1.37E-12	4.00E-16	109543.89	7.5388559	916996.53
1	1320690.183	-4096.048	7.3891015	-0.0028078	7.83E-07	-9.31E-11	4.02E-15	135434.73	-27.220209	916996.53
2	4.10E+08	-253807.25	62.398048	-0.006543	3.51E-07	-8.11E-12	5.91E-17	2122867.5	-516.35502	916996.53
Pb-										
0	0	0	2.5	0	0	0	0	17762.261	8.2351321	153881.93
1	0	0	2.5	0	0	0	0	17762.261	8.2351321	153881.93
2	0	0	2.5	0	0	0	0	17762.261	8.2351321	153881.93
PbBr										
0	-2448.102244	-45.615685	4.6909151	-3.77E-04	5.78E-07	-4.07E-10	1.20E-13	6661.1276	5.9873513	64816.771
1	-1525183.022	4384.561	-0.1457494	0.0022431	-4.46E-07	4.65E-11	-1.88E-15	-21685.68	40.837173	64816.771
PbBr2										
0	-6172.76636	-67.832076	7.2731561	-5.99E-04	7.36E-07	-4.74E-10	1.25E-13	-14278.908	-0.6987992	-103908.06
1	-13204.21479	-1.1430749	7.0009725	-4.28E-07	1.02E-10	-1.23E-14	5.97E-19	-14622.138	0.8868583	-103908.06
PbBr3										
0	-11644.2425	-155.51517	10.623173	-0.0013619	1.67E-06	-1.07E-09	2.82E-13	-14782.083	-14.437586	-104010.96
1	-27879.30766	-2.6332651	10.002232	-9.81E-07	2.33E-10	-2.82E-14	1.36E-18	-15569.812	-10.817655	-104010.96
PbBr4										
0	-11764.58199	-256.7167	14.022233	-0.0022241	2.72E-06	-1.74E-09	4.57E-13	-24621.256	-28.820208	-182435.51
1	-38802.1603	-4.3829338	13.003698	-1.62E-06	3.83E-10	-4.63E-14	2.24E-18	-25923.271	-22.877106	-182435.51
PbCL										
0	1788.25795	-149.39616	5.0781434	-0.0011763	1.49E-06	-9.41E-10	2.44E-13	444.68228	2.295933	8818.592
1	-272907.9656	818.12537	3.4805455	6.87E-04	-1.99E-07	2.97E-11	-1.31E-15	-5479.8683	12.878116	8818.592
PbCL+										
0	0	0	3.9604808	0.0022511	-3.56E-06	2.61E-09	-7.19E-13	88421.37	7.5877429	745609.1
1	0	0	4.4591697	9.74E-05	-4.88E-09	-2.55E-12	6.25E-16	88325.847	5.2131007	745609.1
PbCL2										
0	2830.580143	-313.42567	8.2128273	-0.0025851	3.11E-06	-1.97E-09	5.12E-13	-21675.69	-9.2194155	-175547.47
1	-31491.92744	-5.5654776	7.0045995	-1.99E-06	4.65E-10	-5.58E-14	2.68E-18	-23274.393	-2.1407425	-175547.47
PbCL2+										
0	0	0	5.5653876	0.0057468	-9.24E-06	6.73E-09	-1.83E-12	96334.985	5.249054	816322.64
1	0	0	6.8418837	1.98E-04	-9.66E-08	2.01E-11	-1.32E-15	96094.018	-0.8160435	816322.64
PbCL3										
0	862.358897	-525.31528	12.033363	-0.0043352	5.22E-06	-3.31E-09	8.60E-13	-21805.764	-26.942074	-177653.51
1	-56644.1279	-9.3295148	10.007711	-3.33E-06	7.80E-10	-9.35E-14	4.49E-18	-24485.086	-15.074913	-177653.51
PbCL4										
0	17394.05796	-890.21393	16.375651	-0.007089	8.43E-06	-5.31E-09	1.37E-12	-38882.156	-48.501343	-327430.36
1	-82666.7956	-16.394864	13.013367	-5.72E-06	1.33E-09	-1.59E-13	7.58E-18	-43439.842	-28.745598	-327430.36

PbF										
0	27740.46901	-488.18275	6.0944884	-0.0029288	3.25E-06	-1.92E-09	4.77E-13	-10728.463	-5.3966681	-98867.294
1	-1466759.94	4097.8881	0.1927628	0.0020317	-3.76E-07	3.37E-11	-9.97E-16	-39665.084	35.530614	-98867.294
PbF2										
0	59205.5228	-1052.5293	10.289693	-0.0058763	6.10E-06	-3.42E-09	8.02E-13	-49990.5	-25.251155	-443427.39
1	-85058.9977	-30.742443	7.023346	-9.46E-06	2.11E-09	-2.43E-13	1.13E-17	-55522.368	-5.4960732	-443427.39
PbF3										
0	85530.9087	-1731.0367	15.565962	-0.0102223	1.09E-05	-6.27E-09	1.50E-12	-53003.357	-53.357335	-489572.61
1	-145970.4258	-48.203964	10.036858	-1.50E-05	3.36E-09	-3.90E-13	1.82E-17	-62068.696	-20.069787	-489572.61
PbF4										
0	130996.3563	-2307.2995	19.452014	-0.0102452	9.40E-06	-4.63E-09	9.45E-13	-88041.475	-75.246458	-799925.17
1	-213261.6322	-85.78622	13.064286	-2.58E-05	5.69E-09	-6.53E-13	3.02E-17	-100290.9	-35.902403	-799925.17
PbI										
0	-2400.534472	-19.808575	4.587721	-1.59E-04	3.03E-07	-2.26E-10	7.08E-14	11839.865	7.5437786	108904.21
1	-1778193.642	5244.0092	-1.2983574	0.003023	-7.26E-07	9.47E-11	-4.48E-15	-21723.998	49.823966	108904.21
PbI2										
0	-5904.98672	-48.33307	7.195438	-4.30E-04	5.29E-07	-3.42E-10	8.99E-14	-3107.7802	1.3247737	-10252.63
1	-10883.39477	-0.8164418	7.0006973	-3.08E-07	7.33E-11	-8.90E-15	4.31E-19	-3352.0964	2.4586055	-10252.63
PbI3										
0	-10149.96331	-59.380782	10.240738	-5.30E-04	6.54E-07	-4.23E-10	1.11E-13	-113.84824	-8.9755405	21755.412
1	-16242.29573	-1.0029456	10.000858	-3.80E-07	9.05E-11	-1.10E-14	5.33E-19	-413.82589	-7.5794171	21755.412
PbI4										
0	-12170.96972	-72.263174	13.292942	-6.45E-04	7.96E-07	-5.14E-10	1.35E-13	-8528.1487	-20.104575	-41226.459
1	-19584.77744	-1.2233852	13.001047	-4.63E-07	1.10E-10	-1.34E-14	6.50E-19	-8893.1932	-18.405703	-41226.459
PbO										
0	36437.3438	-451.42927	4.896703	9.64E-04	-2.50E-06	2.19E-09	-6.79E-13	9404.4768	-0.532132	68136.508
1	-975244.871	3949.629	-2.1704569	0.0055369	-2.32E-06	4.62E-10	-3.08E-14	-16987.115	47.929952	68136.508
PbO2										
0	70710.5829	-1076.7575	9.4017117	-0.0010039	-1.23E-06	1.86E-09	-6.83E-13	19996.46	-25.039767	136152.73
1	-130779.667	-73.143615	7.5540834	-2.14E-05	4.70E-09	-5.34E-13	2.46E-17	14133.861	-12.526849	136152.73
PbS										
0	16806.55959	-365.73192	5.8020409	-0.0025673	2.99E-06	-1.83E-09	4.60E-13	15889.607	-3.3037677	127945.52
1	749233.958	-682.27117	2.550167	0.0034034	-1.94E-06	4.58E-10	-3.35E-14	20244.465	15.062788	127945.52
PbS2										
0	24463.7588	-665.48555	9.9202012	-0.0049242	5.72E-06	-3.53E-09	8.97E-13	30443.101	-22.957644	244049.01
1	-54167.003	-13.436003	7.5107004	-4.50E-06	1.03E-09	-1.22E-13	5.79E-18	27012.295	-8.714607	244049.01
Pb2										
0	-843.377073	-21.57963	4.6255417	-2.69E-04	6.73E-07	-5.93E-10	2.17E-13	35498.43	7.0175073	305561.15
1	-1.42E+07	39934.479	-36.424607	0.0185831	-3.49E-06	2.72E-10	-5.90E-15	-221909.57	306.41313	305561.15
Rb										
0	13.52856616	-0.2042233	2.5012138	-3.65E-06	5.88E-09	-4.84E-12	1.60E-15	8985.5692	6.2070055	80900
1	-1138274.064	3804.0419	-2.7508993	0.0038915	-1.63E-06	3.51E-10	-2.52E-14	-14664.548	42.534424	80900
2	3.25E+08	-349385.09	115.90977	-0.0149284	9.58E-07	-3.00E-11	3.66E-16	2636178	-958.65172	80900
Rb+										
0	0	0	2.5	0	0	0	0	58203.274	5.5205069	490129.13
1	0	0	2.5	0	0	0	0	58203.274	5.5205069	490129.13
2	4.12E+07	-29203.765	11.020968	-0.0013115	1.12E-07	-5.11E-12	9.62E-17	285016.61	-66.722023	490129.13
Rb-										
0	0	0	2.5	0	0	0	0	2600.4058	5.5205262	27818.528
1	0	0	2.5	0	0	0	0	2600.4058	5.5205262	27818.528
2	0	0	2.5	0	0	0	0	2600.4058	5.5205262	27818.528
RbOH										
0	12138.32721	-544.14116	8.4598146	-0.0035615	2.99E-06	-7.28E-10	-4.55E-14	-27872.625	-19.13422	-238000
1	895858.313	-2332.339	7.9711925	1.04E-04	-6.33E-08	1.03E-11	-5.74E-16	-15155.689	-19.500516	-238000
Rb2O2H2										
0	-4577.07653	-841.7631	17.040838	-0.0053579	3.95E-06	-2.05E-10	-4.09E-13	-76949.822	-54.354128	-639000
1	1792711.652	-4659.4066	16.938224	2.11E-04	-1.27E-07	2.06E-11	-1.15E-15	-50241.176	-60.270549	-639000
Rn										
0	3.39E-06	-1.31E-07	2.5	-2.98E-12	4.34E-15	-3.18E-18	9.25E-22	-745.375	6.952442	0
1	27301.90029	-82.846726	2.5981785	-5.81E-05	1.82E-08	-2.87E-12	1.79E-16	-220.28093	6.2550057	0
2	9.18E+08	-624585.46	172.49465	-0.0232576	1.64E-06	-5.37E-11	6.51E-16	4883105.9	-1449.5161	0
Rn+										
0	-0.09697149	0.0011067	2.4999949	1.19E-08	-1.52E-11	9.96E-15	-2.64E-18	124730.48	8.3387617	1043270.3
1	-19982.85319	59.306757	2.432476	3.72E-05	-1.01E-08	1.19E-12	-3.18E-17	124352.85	8.8219978	1043270.3
2	-2.41E+07	15711.517	-1.4116838	4.50E-04	-2.32E-08	5.83E-13	-5.82E-18	918.74575	42.336133	1043270.3
S										
0	-317.484182	-192.47049	4.6868259	-0.0058414	7.54E-06	-4.86E-09	1.26E-12	33235.922	-5.7184772	277170
1	-485424.479	1438.8304	1.2585041	3.80E-04	1.63E-09	-9.55E-12	8.04E-16	23349.953	15.595595	277170
2	-1.30E+08	69093.62	-11.76228	0.0016015	-1.05E-07	4.34E-12	-7.68E-17	-526148.5	132.21957	277170
S+										
0	0	0	2.5	0	0	0	0	153502.61	5.4362701	1282496.4
1	1346218.684	-4056.8715	7.1534366	-0.0025236	6.43E-07	-6.43E-11	2.14E-15	179282.38	-27.869304	1282496.4
2	1.54E+08	-102307.35	25.917969	-0.0021115	9.22E-08	-1.96E-12	2.10E-17	962241.84	-201.72395	1282496.4
S-										
0	-2596.051473	-142.23987	4.0078257	-0.0036089	4.24E-06	-2.52E-09	6.08E-13	8197.7931	-2.5823306	70368.505
1	2730.311692	141.40721	2.4033408	3.69E-05	-7.94E-09	8.95E-13	-4.10E-17	6931.1957	6.5750337	70368.505
2	-122368.2088	120.31258	2.4739423	2.94E-06	-1.81E-10	5.78E-15	-7.49E-20	6947.8412	6.0706266	70368.505
SCL										
0	0	0	3.705588	0.0052719	-1.14E-05	1.05E-08	-3.53E-12	17561.159	6.2794512	156469.99
1	0	0	4.594726	-5.98E-05	4.52E-08	-9.37E-12	8.07E-16	17452.426	2.3798515	156469.99
SCL2										
0	0	0	3.5966371	0.0143272	-2.52E-05	2.06E-08	-6.40E-12	-3637.5837	10.060556	-17572.262

1	0	0	6.6271462	4.27E-04	-1.88E-07	3.58E-11	-2.38E-15	-4200.0219	-4.2323703	-17572.262
SCL2+										
0	0	0	3.5958727	0.0142917	-2.51E-05	2.04E-08	-6.35E-12	106902.83	10.755834	901508.6
1	0	0	6.580257	5.22E-04	-2.51E-07	5.10E-11	-3.27E-15	106354.86	-3.2949383	901508.6
SD										
0	0	0	4.7285597	-0.005094	9.91E-06	-7.33E-09	1.95E-12	15399.579	-1.5684795	138494.85
1	0	0	3.3471988	0.001213	-4.77E-07	8.83E-11	-6.07E-15	15627.147	4.877642	138494.85
SF										
0	12064.5668	-291.02707	5.4801015	-0.0019759	2.47E-06	-1.61E-09	4.31E-13	1991.3375	-4.5441093	15445.561
1	763456.24	-2423.6339	7.3521944	-0.001598	4.87E-07	-6.48E-11	2.98E-15	15774.586	-19.025788	15445.561
SF+										
0	0	0	2.6666648	0.0056975	-7.61E-06	4.91E-09	-1.24E-12	118310.33	10.515019	991925.69
1	0	0	4.2807248	1.04E-04	5.54E-08	-1.14E-11	5.58E-16	117921.92	2.4593947	991925.69
SF-										
0	50198.7928	-532.15493	4.904849	9.92E-04	-2.27E-06	1.84E-09	-5.36E-13	-26113.886	-3.6374387	-231346.89
1	206892.3125	-1324.3728	6.6462112	-0.0016418	6.78E-07	-1.20E-10	7.12E-15	-21509.948	-14.702362	-231346.89
SF2										
0	68705.3997	-843.19612	6.2692529	0.0064848	-1.15E-05	8.77E-09	-2.54E-12	-32300.028	-8.7986397	-293188.73
1	-170335.58	-149.4915	7.1107005	-4.40E-05	9.65E-09	-1.10E-12	5.07E-17	-37044.255	-10.95084	-293188.73
SF2+										
0	0	0	2.427149	0.0155175	-2.31E-05	1.65E-08	-4.62E-12	83239.557	14.127887	702406.52
1	0	0	6.1209	1.00E-03	-4.40E-07	8.44E-11	-5.78E-15	82444.585	-3.8630754	702406.52
SF2-										
0	0	0	3.2900503	0.0155386	-2.72E-05	2.22E-08	-6.89E-12	-49391.925	9.8174776	-398434.66
1	0	0	6.5847123	4.79E-04	-2.14E-07	4.22E-11	-3.05E-15	-50005.705	-5.7333479	-398434.66
SF3										
0	128400.104	-2084.8586	14.234125	-0.0040147	9.15E-07	1.11E-09	-5.99E-13	-52395.232	-51.87147	-504101.4
1	-241094.039	-141.98164	10.105989	-4.24E-05	9.35E-09	-1.07E-12	4.95E-17	-63583.893	-24.896215	-504101.4
SF3+										
0	0	0	1.0018508	0.0297552	-4.34E-05	3.06E-08	-8.46E-12	46044.184	19.444501	393598.44
1	0	0	8.1385016	0.0021289	-9.48E-07	1.86E-10	-1.33E-14	44486.73	-15.421242	393598.44
SF3-										
0	154650.0675	-2469.7685	16.575485	-0.0102014	9.37E-06	-4.73E-09	1.01E-12	-85001.579	-65.321648	-790124.21
1	-225386.0964	-130.88902	10.099724	-4.05E-05	9.06E-09	-1.05E-12	4.90E-17	-98002.272	-25.243663	-790124.21
SF4										
0	163620.231	-2531.3482	15.591274	0.003326	-1.05E-05	9.39E-09	-2.91E-12	-81155.441	-61.316442	-760000
1	-377653.292	-293.93337	13.219218	-8.76E-05	1.93E-08	-2.21E-12	1.02E-16	-94830.646	-42.432014	-760000
SF4+										
0	0	0	1.9615813	0.0421321	-6.92E-05	5.37E-08	-1.61E-11	48094.74	16.379901	416056.41
1	0	0	11.351941	0.0018876	-8.39E-07	1.64E-10	-1.17E-14	46224.767	-28.571508	416056.41
SF4-										
0	0	0	4.0793762	0.0378395	-6.69E-05	5.48E-08	-1.71E-11	-109146.42	5.6417878	-887483.61
1	0	0	12.003326	0.0012008	-5.74E-07	1.23E-10	-9.30E-15	-110603.08	-31.659265	-887483.61
SF5										
0	222422.006	-4044.0563	27.072347	-0.0174429	1.60E-05	-8.00E-09	1.67E-12	-92200.477	-123.2447	-902663.29
1	-389387.925	-182.17658	16.137213	-5.52E-05	1.22E-08	-1.41E-12	6.53E-17	-113569.72	-55.772077	-902663.29
SF5+										
0	0	0	-1.7164861	0.06894	-1.15E-04	9.00E-08	-2.72E-11	19061.149	29.444513	172651.43
1	0	0	13.684216	0.0025177	-1.09E-06	2.25E-10	-1.72E-14	16004.908	-44.199724	172651.43
SF5-										
0	209503.1134	-3930.0811	27.021272	-0.0179297	1.72E-05	-9.00E-09	1.99E-12	-129181.66	-123.16727	-1204622.3
1	-373321.92	-179.37295	16.136997	-5.58E-05	1.25E-08	-1.45E-12	6.77E-17	-149855.44	-56.314382	-1204622.3
SF6										
0	330944.792	-4737.5788	22.476832	0.0104709	-2.56E-05	2.15E-08	-6.52E-12	-125536.57	-109.17291	-1219400
1	-730673.374	-636.69917	19.474418	-1.89E-04	4.18E-08	-4.78E-12	2.21E-16	-151061.02	-81.475661	-1219400
SF6-										
0	0	0	-3.2609272	0.0826954	-1.33E-04	1.02E-07	-3.01E-11	-163108.6	35.423344	-1341907.9
1	0	0	15.428646	0.0040845	-1.82E-06	3.57E-10	-2.58E-14	-166898.84	-54.396122	-1341907.9
SH										
0	6389.43468	-374.79609	7.5481458	-0.0128888	1.91E-05	-1.27E-08	3.24E-12	17221.772	-17.607573	140412.11
1	1682631.601	-5177.1522	9.1981685	-0.0023236	6.54E-07	-8.47E-11	3.86E-15	48784.893	-37.703957	140412.11
SH-										
0	38780.7076	-574.25906	6.8985445	-0.0100135	1.49E-05	-9.75E-09	2.45E-12	-8942.6411	-16.15962	-88297.296
1	1198715.402	-3894.8468	7.6604223	-0.0013552	3.34E-07	-3.35E-11	9.06E-16	12967.522	-28.183661	-88297.296
SN										
0	-68354.1235	1147.5675	-2.8778026	0.0172486	-2.06E-05	1.26E-08	-3.14E-12	25641.436	42.240104	267388.31
1	-483728.446	1058.0756	3.0861988	9.11E-04	-2.76E-07	4.16E-11	-2.13E-15	23793.455	10.332255	267388.31
SO										
0	-33427.57	640.38625	-1.0066412	0.0138151	-1.70E-05	1.06E-08	-2.65E-12	-3371.2922	30.938651	4760.306
1	-1443410.557	4113.8744	-0.5383696	0.0027942	-6.63E-07	7.84E-11	-3.56E-15	-27088.381	36.153615	4760.306
SO-										
0	8420.19697	-69.165867	3.8376666	0.0021665	-2.81E-06	1.79E-09	-4.52E-13	-13541.625	4.3161728	-105968.09
1	176715.6147	-663.39874	5.1772798	-2.85E-04	7.21E-08	-3.68E-12	-2.91E-16	-9984.438	-3.9514256	-105968.09
SOF2										
0	61142.8667	-908.06973	6.8833855	0.0119253	-1.67E-05	1.11E-08	-2.91E-12	-67429.56	-11.253252	-584952.31
1	-251140.931	-607.20079	10.4502	-1.79E-04	3.96E-08	-4.54E-12	2.10E-16	-70722.275	-29.041407	-584952.31
SO2										
0	-53108.4214	909.03117	-2.3568912	0.0220445	-2.51E-05	1.45E-08	-3.37E-12	-41137.521	40.455149	-296810
1	-112764.0116	-825.22614	7.6161786	-2.00E-04	5.66E-08	-5.45E-12	2.92E-16	-33513.087	-16.557737	-296810
SO2-										
0	94609.0166	-856.26911	5.3600742	0.0076096	-1.09E-05	7.20E-09	-1.85E-12	-45800.948	-3.9299332	-408606.07
1	-179340.0005	-366.31688	7.2744411	-1.10E-04	2.44E-08	-2.81E-12	1.31E-16	-49730.726	-12.614188	-408606.07

SO2CLF										
0	0	0	2.9817528	0.0264492	-2.92E-05	1.40E-08	-2.03E-12	-68761.497	12.731681	-556475.7
1	0	0	10.118286	0.0031489	-1.35E-06	2.56E-10	-1.79E-14	-70509.291	-23.127851	-556475.7
SO2CL2										
0	0	0	4.3851677	0.0232122	-2.65E-05	1.35E-08	-2.28E-12	-44802.974	6.5786788	-354802.07
1	0	0	10.550937	0.0026734	-1.14E-06	2.17E-10	-1.52E-14	-46295.056	-24.307857	-354802.07
SO2F2										
0	55331.9117	-807.4694	5.2872033	0.0229454	-2.89E-05	1.79E-08	-4.42E-12	-88994.262	-4.1244136	-760000
1	-340327.569	-1309.4778	13.966233	-3.84E-04	8.46E-08	-9.68E-12	4.48E-16	-89018.74	-51.09424	-760000
SO3										
0	-39530.5842	620.88564	-1.4378852	0.0276417	-3.15E-05	1.79E-08	-4.13E-12	-51841.198	33.914189	-395900
1	-216640.492	-1301.1815	10.963065	-3.84E-04	8.47E-08	-9.71E-12	4.50E-16	-43981.831	-36.553476	-395900
S2										
0	35280.9178	-422.21566	4.6774335	0.001724	-3.86E-06	3.34E-09	-9.93E-13	16547.677	-0.7956811	128600
1	-15881.28788	631.54809	2.4496281	0.0019862	-6.51E-07	1.00E-10	-5.60E-15	10855.084	14.585492	128600
S2-										
0	10255.58251	-616.61283	8.1820528	-0.0083112	9.72E-06	-5.78E-09	1.39E-12	-3063.5599	-19.060634	-37132.385
1	483020.403	-1319.1713	6.0317785	-7.97E-04	2.28E-07	-2.50E-11	7.28E-16	2660.2585	-9.0104335	-37132.385
S2CL2										
0	0	0	3.4790571	0.032537	-6.64E-05	6.21E-08	-2.17E-11	-4022.2557	12.279182	-16736
1	0	0	9.4684102	0.0011219	-6.93E-07	1.39E-10	-9.29E-15	-5050.1952	-15.295044	-16736
S2F2,thiothony										
0	125290.4041	-1941.2439	13.253822	-0.0013415	-2.77E-06	3.66E-09	-1.30E-12	-40672.083	-45.608257	-401413
1	-259175.7719	-105.96531	10.065886	-2.27E-05	5.41E-09	-9.91E-13	9.62E-17	-51476.752	-23.756632	-401413
S2O										
0	10927.0331	-95.230999	3.1445254	0.0117685	-1.58E-05	1.04E-08	-2.71E-12	-7500.4719	11.041736	-56035.495
1	-144213.979	-327.64301	7.2442861	-9.78E-05	2.16E-08	-2.48E-12	1.15E-16	-7438.5539	-10.85177	-56035.495
S3										
0	72454.0366	-1162.148	9.9554217	-0.0041581	3.24E-06	-1.26E-09	1.78E-13	21462.761	-25.875256	144738.33
1	-111782.01	-51.98656	7.0387819	-1.55E-05	3.42E-09	-3.91E-13	1.81E-17	15254.101	-7.6101374	144738.33
S4										
0	119867.386	-2040.7987	15.102408	-0.0070412	5.35E-06	-2.00E-09	2.57E-13	24109.154	-55.031814	135632.33
1	-206858.571	-96.888596	10.072349	-2.89E-05	6.37E-09	-7.29E-13	3.37E-17	13210.63	-23.448085	135632.33
S5										
0	136139.136	-2955.5028	26.33371	-0.0412583	7.06E-05	-5.61E-08	1.66E-11	26753.201	-106.97176	132993.35
1	-4038678.25	8602.2873	7.4432874	0.0015336	-2.53E-07	2.15E-11	-7.22E-16	-46872.388	11.045918	132993.35
S6										
0	97820.3226	-2568.7152	24.671612	-0.0162036	1.71E-05	-9.75E-09	2.49E-12	20380.06	-101.44853	101315.18
1	3686830.92	-7694.9761	18.607177	0.0022904	-1.22E-06	2.06E-10	-1.19E-14	60324.596	-74.902097	101315.18
S7										
0	123358.23	-3200.4349	30.156164	-0.021973	2.49E-05	-1.51E-08	3.77E-12	23899.542	-127.59431	111890.37
1	-272698.953	-73.550394	19.057508	-2.38E-05	5.41E-09	-6.33E-13	2.99E-17	7307.3062	-61.589568	111890.37
S8										
0	314537.784	-6116.1635	48.751401	-0.0624129	7.42E-05	-3.73E-08	5.80E-12	35737.239	-228.85968	101277.12
1	-8728336.09	12217.389	22.098434	-0.0034935	1.40E-06	-2.17E-10	1.21E-14	-86588.281	-64.348986	101277.12
Sc										
0	-3700.80594	169.2506	1.8422426	0.0013648	-1.58E-06	9.61E-10	-2.39E-13	43852.152	10.727819	377700.26
1	8810382.65	-27112.33	34.765887	-0.018611	5.29E-06	-6.59E-10	3.00E-14	216246.01	-222.56185	377700.26
2	2.28E+09	-1367701.2	321.35931	-0.0356317	2.09E-06	-6.24E-11	7.43E-16	1.09E+07	-2781.4094	377700.26
Sc+										
0	-5884.93016	147.90444	2.0095765	7.39E-04	-6.62E-07	6.84E-10	-2.16E-13	120843.91	10.265706	1017145.2
1	1973658.531	-4954.3841	6.3606274	-7.17E-04	2.46E-08	9.63E-12	-8.54E-16	154342.38	-22.619258	1017145.2
2	2.22E+08	-128788.14	32.655939	-0.00338	1.98E-07	-5.19E-12	4.64E-17	1149364.3	-255.32949	1017145.2
Sc-										
0	0	0	2.5	0	0	0	0	41657.464	8.2704207	352558.83
1	0	0	2.5	0	0	0	0	41657.464	8.2704207	352558.83
2	0	0	2.5	0	0	0	0	41657.464	8.2704207	352558.83
Si										
0	98.3614081	154.65445	1.8764367	0.0013206	-1.53E-06	8.95E-10	-1.95E-13	52635.103	9.6982889	450000
1	-616929.885	2240.6839	-0.4448619	0.0017101	-4.11E-07	4.56E-11	-1.89E-15	39535.588	26.796681	450000
2	-9.29E+08	544398.99	-120.67397	0.0135966	-7.61E-07	2.15E-11	-2.47E-16	-4293792.1	1086.3828	450000
Si+										
0	-43297.9188	679.58945	0.2257046	0.0041186	-4.23E-06	2.33E-09	-5.32E-13	145203.98	19.346505	1242508
1	59193.9023	-48.56731	2.556312	-3.50E-05	1.19E-08	-2.08E-12	1.47E-16	149143.14	5.2442671	1242508
2	-1.36E+07	7022.7772	1.23301	1.21E-04	-1.46E-08	1.53E-12	-3.80E-17	91492.381	17.083378	1242508
Si-										
0	-794.014667	5.5674184	2.4998372	-9.48E-05	3.17E-07	-4.19E-10	2.04E-13	36364.434	5.2701198	308817.53
1	-6162070.1	18833.104	-18.993025	0.0111102	-2.54E-06	2.70E-10	-1.11E-14	-83140.893	159.52983	308817.53
2	-5.43E+07	32971.057	-2.4705797	3.97E-04	-1.76E-08	4.12E-13	-3.90E-18	-231588.15	52.266018	308817.53
SiBr										
0	7370.28335	-505.1063	8.280591	-0.0100538	1.36E-05	-9.12E-09	2.45E-12	21844.055	-16.620327	175157.42
1	1317799.94	-3669.795	8.5116861	-0.0019876	5.04E-07	-4.49E-11	8.24E-16	43328.516	-24.670755	175157.42
SiBr2										
0	23863.4484	-641.53097	9.3456683	-0.0047923	5.58E-06	-3.45E-09	8.80E-13	-5014.9414	-17.406502	-51000
1	-51434.3821	-12.913443	7.0103762	-4.40E-06	1.02E-09	-1.21E-13	5.79E-18	-8318.6934	-3.6130552	-51000
SiBr3										
0	39733.6999	-1066.5458	13.80869	-0.0076418	8.78E-06	-5.37E-09	1.36E-12	-16517.606	-37.842445	-157000
1	-88884.959	-22.673611	10.017916	-7.49E-06	1.71E-09	-2.02E-13	9.55E-18	-22030.311	-15.375764	-157000
SiBr4										
0	68198.1596	-1520.1827	18.103441	-0.0097315	1.07E-05	-6.34E-09	1.56E-12	-46166.746	-59.755186	-415800
1	-127317.783	-37.191681	13.028577	-1.17E-05	2.61E-09	-3.02E-13	1.41E-17	-54093.134	-29.400037	-415800
SiC										

0	-6223.33089	314.17905	0.3893131	0.0118751	-1.64E-05	1.13E-08	-3.05E-12	86062.277	23.101645	734946.14
1	-62688.0603	720.98369	2.1628797	0.0022013	-6.57E-07	9.18E-11	-4.97E-15	83212.259	16.016731	734946.14
SiC2										
0	-41196.584	686.97908	0.0235876	0.0153295	-1.44E-05	6.38E-09	-1.06E-12	71308.886	28.288628	631360.94
1	7026787.99	-24661.186	39.154203	-0.0200287	6.31E-06	-8.85E-10	4.53E-14	226730.6	-236.65987	631360.94
SiC4H12										
0	0	0	4.9461863	0.041143	-2.93E-07	-2.29E-08	1.10E-11	-37731.049	3.1862702	-286604
1	0	0	11.563702	0.0328112	-1.26E-05	2.27E-09	-1.54E-13	-40138.137	-33.63416	-286604
SiCL										
0	13467.6349	-217.04907	5.034083	-6.57E-04	4.84E-07	-1.40E-10	4.31E-15	16928.012	-0.5641114	142360.25
1	-257161.466	729.2137	3.6024491	5.93E-04	-1.69E-07	2.47E-11	-1.10E-15	11105.135	9.1593065	142360.25
SiCL2										
0	53051.4405	-1015.7822	10.328128	-0.0062112	6.71E-06	-3.91E-09	9.46E-13	-16502.469	-26.497319	-163069.29
1	-80486.8555	-26.689703	7.0205201	-8.40E-06	1.89E-09	-2.20E-13	1.04E-17	-21812.457	-6.6395132	-163069.29
SiCL3										
0	86908.6184	-1677.432	15.114474	-0.008935	9.09E-06	-5.01E-09	1.16E-12	-34775.367	-50.868202	-336271.67
1	-147697.778	-53.425705	10.040539	-1.64E-05	3.67E-09	-4.24E-13	1.98E-17	-43605.263	-20.067055	-336271.67
SiCL4										
0	117175.236	-2185.9736	19.08336	-0.0096388	8.84E-06	-4.36E-09	8.95E-13	-72127.293	-73.020073	-662200
1	-210253.576	-84.152309	13.063	-2.52E-05	5.57E-09	-6.37E-13	2.95E-17	-83726.605	-35.921228	-662200
SiF										
0	13435.19512	33.41197	2.2091423	0.0074553	-1.07E-05	7.52E-09	-2.07E-12	-4089.1227	12.945983	-25231.846
1	-180980.8236	289.73324	4.1028636	2.87E-04	-8.05E-08	1.19E-11	-5.05E-16	-6450.4496	3.8527665	-25231.846
SiFCL										
0	41770.8011	-592.67604	6.4098774	0.0046414	-7.98E-06	6.01E-09	-1.72E-12	-43982.774	-6.2603315	-377825.7
1	-128461.539	-124.7806	7.0929223	-3.71E-05	8.18E-09	-9.36E-13	4.33E-17	-47232.836	-8.3376032	-377825.7
SiF2										
0	40530.3549	-399.73439	4.0551353	0.0115347	-1.76E-05	1.26E-08	-3.52E-12	-70477.845	3.8807851	-592838.11
1	-167529.644	-184.59769	7.136966	-5.45E-05	1.20E-08	-1.37E-12	6.33E-17	-72874.165	-11.179181	-592838.11
SiF3										
0	57550.9603	-717.92116	5.3791863	0.0181312	-2.74E-05	1.95E-08	-5.39E-12	-117763.3	-3.4417292	-996436.58
1	-290365.855	-342.68077	10.255247	-1.02E-04	2.25E-08	-2.58E-12	1.19E-16	-121809.58	-27.251772	-996436.58
SiF4										
0	12407.7408	-123.57875	2.6830035	0.0326735	-4.55E-05	3.09E-08	-8.27E-12	-195400.01	10.402945	-1615000
1	-387374.88	-629.67814	13.47017	-1.88E-04	4.16E-08	-4.78E-12	2.22E-16	-195789.58	-46.523132	-1615000
SiH										
0	-2665.600539	29.246113	4.2101471	-0.0047801	1.11E-05	-9.23E-09	2.75E-12	43046.687	0.921133	368718.36
1	-1470883.237	3710.0351	-0.0880599	0.0023753	-4.78E-07	4.84E-11	-1.75E-15	18969.663	29.797585	368718.36
SiH+										
0	0	0	3.7292588	-0.0017882	4.25E-06	-2.56E-09	4.06E-13	136970.71	1.5838731	1147699.8
1	0	0	2.9828595	0.0015455	-5.90E-07	1.05E-10	-6.82E-15	137079.54	5.0403501	1147699.8
SiHBr3										
0	0	0	4.337011	0.028873	-4.70E-05	3.75E-08	-1.16E-11	-38663.834	10.321671	-302927.68
1	0	0	10.274831	0.0028666	-1.21E-06	2.30E-10	-1.62E-14	-39846.576	-18.034066	-302927.68
SiHCL										
0	59096.7305	-878.0064	7.9996879	-0.0046631	8.59E-06	-6.61E-09	1.87E-12	9567.5703	-16.90015	54945.913
1	101215.289	-1163.2396	7.3763666	1.87E-04	-1.66E-07	3.96E-11	-2.64E-15	11410.641	-15.076795	54945.913
SiHCL3										
0	0	0	2.6742042	0.0343804	-5.50E-05	4.31E-08	-1.32E-11	-61601.723	14.33351	-496233.68
1	0	0	9.9335635	0.0032481	-1.38E-06	2.63E-10	-1.86E-14	-63070.849	-20.472059	-496233.68
SiHF										
0	21925.98671	-61.752291	2.1273727	0.0112354	-1.32E-05	8.31E-09	-2.01E-12	-20169.948	13.671849	-162657.17
1	4049752.24	-9295.5268	10.717544	0.0018681	-1.13E-06	1.96E-10	-1.14E-14	41332.252	-47.363176	-162657.17
SiHF3										
0	0	0	0.9065482	0.0332653	-4.39E-05	2.93E-08	-7.86E-12	-145841.96	19.973266	-1200839.7
1	0	0	8.7548828	0.0045528	-1.95E-06	3.73E-10	-2.65E-14	-147656.58	-18.826977	-1200839.7
SiHI3										
0	0	0	5.5211225	0.0248411	-4.08E-05	3.31E-08	-1.04E-11	-11407.189	7.7846695	-74475.337
1	0	0	10.533604	0.0025888	-1.09E-06	2.07E-10	-1.46E-14	-12397.345	-16.095034	-74475.337
SiH2										
0	-195834.112	2758.775	-9.908961	0.0276317	-1.03E-05	-9.05E-09	5.89E-12	18333.442	81.858894	273350.22
1	-2005373.278	3817.5633	4.1581256	0.001035	-2.06E-07	2.28E-11	-1.06E-15	3984.8238	4.8362727	273350.22
SiH2Br2										
0	0	0	2.0007427	0.0302826	-4.47E-05	3.44E-08	-1.05E-11	-24507.507	18.566737	-190375.71
1	0	0	8.1692601	0.0050286	-2.11E-06	3.99E-10	-2.80E-14	-25842.475	-11.371191	-190375.71
SiH2CL2										
0	0	0	1.0264938	0.0330136	-4.80E-05	3.62E-08	-1.09E-11	-39963.387	20.628857	-320501.8
1	0	0	7.9121404	0.0053128	-2.23E-06	4.23E-10	-2.98E-14	-41468.503	-12.886763	-320501.8
SiH2F2										
0	0	0	0.19376	0.0300799	-3.59E-05	2.27E-08	-5.92E-12	-96230.327	22.860754	-790797.57
1	0	0	7.0981857	0.0062146	-2.63E-06	4.99E-10	-3.52E-14	-97918.745	-11.672569	-790797.57
SiH2I2										
0	0	0	2.6562813	0.0286262	-4.30E-05	3.37E-08	-1.05E-11	-6325.2612	17.270925	-38073.923
1	0	0	8.3573099	0.0048164	-2.02E-06	3.80E-10	-2.67E-14	-7541.7667	-10.297355	-38073.923
SiH3										
0	4341.14282	227.71851	0.650825	0.0122144	-4.35E-06	-1.77E-09	1.18E-12	22599.938	19.683475	204357.37
1	605632.122	-4721.2541	13.291295	-0.0012568	2.69E-07	-3.01E-11	1.37E-15	49744.206	-61.405031	204357.37
SiH3Br										
0	0	0	1.0060335	0.0253079	-3.04E-05	2.11E-08	-6.21E-12	-10605.36	19.467545	-78242.643
1	0	0	6.1350363	0.0071113	-2.97E-06	5.61E-10	-3.94E-14	-11879.9	-6.1782657	-78242.643
SiH3CL										
0	0	0	0.5830799	0.0261617	-3.09E-05	2.09E-08	-6.02E-12	-18161.979	20.236538	-141841.39

1	0	0	5.9919718	0.0072719	-3.04E-06	5.74E-10	-4.03E-14	-19514.93	-6.8676437	-141841.39
SiH3F										
0	0	0	0.3736973	0.023371	-2.19E-05	1.14E-08	-2.62E-12	-46268.676	20.45413	-376571.11
1	0	0	5.5736119	0.007741	-3.25E-06	6.15E-10	-4.32E-14	-47688.486	-6.2100229	-376571.11
SiH3I										
0	0	0	1.365932	0.0245926	-3.00E-05	2.12E-08	-6.35E-12	-1525.8355	18.640398	-2091.662
1	0	0	6.2686663	0.0069652	-2.91E-06	5.48E-10	-3.85E-14	-2737.3527	-5.8284516	-2091.662
SiH4										
0	78730.7459	-552.62209	2.4990293	0.0144209	-8.47E-06	2.73E-09	-5.44E-13	6269.7313	4.9650001	34700
1	1290384.93	-7813.4308	18.288563	-0.0019757	4.16E-07	-4.60E-11	2.07E-15	47669.066	-98.017294	34700
SiI										
0	96614.2672	-1598.809	12.52071	-0.0163387	1.75E-05	-9.66E-09	2.18E-12	37915.788	-41.448017	262953.59
1	-344203.091	1314.2663	3.1423341	7.51E-04	-1.67E-07	9.95E-12	1.85E-15	22096.086	15.098325	262953.59
SiI2										
0	0	0	4.3215511	0.0144273	-3.11E-05	2.98E-08	-1.06E-11	9412.182	10.817857	92470
1	0	0	6.7431186	3.62E-04	-1.95E-07	4.36E-11	-2.90E-15	9069.7536	0.0129097	92470
SiN										
0	-14646.72152	137.49935	3.6785086	-0.0061585	2.31E-05	-2.29E-08	7.40E-12	46732.13	6.4945655	403668.44
1	-2932685.132	5853.6886	1.3214517	0.0012583	-3.77E-07	6.89E-11	-4.19E-15	6527.1488	25.531459	403668.44
SiO										
0	-47227.7105	806.31376	-1.6369761	0.0145428	-1.72E-05	1.04E-08	-2.56E-12	-16665.859	33.557957	-98842.418
1	-176513.4162	-31.991771	4.4774419	4.59E-06	3.56E-08	-1.33E-11	1.61E-15	-13508.424	-0.8386957	-98842.418
SiO2										
0	-33629.4878	473.40789	0.2309771	0.0185023	-2.24E-05	1.36E-08	-3.35E-12	-42264.875	22.958032	-322073.48
1	-146403.1193	-626.14411	7.9645637	-1.85E-04	4.10E-08	-4.70E-12	2.18E-16	-37918.348	-20.452854	-322073.48
SiS										
0	35994.4929	-423.97233	4.6540144	0.0015885	-3.31E-06	2.71E-09	-8.11E-13	14115.156	-1.1831769	108194.41
1	-2102323.897	6228.8362	-3.0041209	0.0044955	-1.37E-06	2.00E-10	-9.88E-15	-27955.382	54.058313	108194.41
SiS2										
0	43977.4566	-743.00131	7.9415884	0.0020381	-4.65E-06	3.85E-09	-1.16E-12	2801.0779	-17.368851	7022.717
1	-126648.9071	-97.742352	7.5728037	-2.91E-05	6.41E-09	-7.33E-13	3.39E-17	-1244.6723	-13.527072	7022.717
Si2										
0	12375.96221	-102.49044	4.3548485	0.0012811	-2.53E-06	2.27E-09	-7.00E-13	69069.429	3.2511252	580195.52
1	1370060.657	-4207.06	9.3374329	-0.0027492	9.59E-07	-1.37E-10	6.77E-15	95108.845	-31.683852	580195.52
Si2C										
0	-4553.61239	131.48234	2.4690973	0.0127652	-1.66E-05	1.07E-08	-2.74E-12	64700.485	14.688442	554093.9
1	-125436.658	-341.27469	7.2541967	-1.02E-04	2.25E-08	-2.58E-12	1.20E-16	66079.113	-11.460961	554093.9
Si2N										
0	0	0	3.6686735	0.0113018	-1.36E-05	7.17E-09	-1.24E-12	46318.083	7.1227096	397494.51
1	0	0	6.6709912	9.19E-04	-3.95E-07	7.44E-11	-5.03E-15	45620.154	-7.7982777	397494.51
Si3										
0	-11142.9441	157.59102	2.4860675	0.0163165	-2.21E-05	1.37E-08	-3.26E-12	73282.479	15.881192	627867.38
1	-1699325.75	4697.6153	2.6184211	0.001959	-2.58E-07	6.10E-12	6.09E-16	42780.448	25.863805	627867.38
Sn										
0	-124869.2263	1618.8412	-4.6023974	0.0104543	3.00E-06	-1.07E-08	4.32E-12	27483.64	48.050672	301200
1	-5145695.64	11405.751	-4.1796321	0.0022364	-3.60E-07	2.44E-11	-2.94E-16	-42150.136	59.814509	301200
2	-1.12E+09	642704.6	-137.86159	0.0145387	-7.11E-07	1.50E-11	-8.94E-17	-5111296.9	1245.6255	301200
Sn+										
0	-5571.29778	122.23232	1.5663614	0.0033971	-6.31E-06	5.59E-09	-1.69E-12	120902.41	11.626348	1015949.9
1	4622916.85	-11859.587	12.370265	-0.0027736	3.10E-07	-5.36E-12	-8.66E-16	199432.3	-68.371083	1015949.9
2	1.91E+08	-114573.02	30.702942	-0.0033879	1.97E-07	-4.39E-12	2.06E-17	1031631.1	-237.01579	1015949.9
Sn-										
0	272279.6	-3369.9358	17.439064	-0.0281053	2.79E-05	-1.44E-08	3.07E-12	37532.278	-80.07857	179495.95
1	-64477.1322	743.05551	1.9213803	2.36E-04	-5.28E-08	6.10E-12	-2.84E-16	16457.394	12.654369	179495.95
2	-1314284.778	897.23543	2.3023545	2.25E-05	-1.39E-09	4.47E-14	-5.81E-19	14288.006	10.049338	179495.95
SnBr										
0	25641.93542	-525.91223	7.6874107	-0.0096542	1.48E-05	-9.94E-09	2.48E-12	10204.839	-11.265504	75644.02
1	1815578.541	-6728.2646	13.324645	-0.0046081	1.24E-06	-1.53E-10	6.97E-15	49255.831	-56.409628	75644.02
SnBr2										
0	-4995.75306	-136.64989	7.5435639	-0.0011818	1.44E-06	-9.25E-10	2.42E-13	-15755.07	-3.595584	-118974.59
1	-19408.94091	-2.3356079	7.0019693	-8.62E-07	2.04E-10	-2.46E-14	1.19E-18	-16448.281	-0.4349355	-118974.59
SnBr3										
0	-8050.41647	-289.79625	11.144434	-0.0024754	3.01E-06	-1.93E-09	5.03E-13	-20700.666	-18.959654	-158716.45
1	-38930.0453	-4.9908442	10.004184	-1.82E-06	4.31E-10	-5.19E-14	2.50E-18	-22172.995	-12.298541	-158716.45
SnBr4										
0	-5832.84092	-427.01985	14.674665	-0.0036043	4.37E-06	-2.79E-09	7.27E-13	-40829.165	-34.471044	-324216.98
1	-51768.1292	-7.426127	13.006195	-2.69E-06	6.34E-10	-7.63E-14	3.67E-18	-43001.663	-24.714551	-324216.98
SnCL										
0	33515.4973	-683.22086	8.3939177	-0.0116443	1.81E-05	-1.26E-08	3.30E-12	6051.7909	-16.678349	34658.816
1	774160.568	-3602.0485	9.7490598	-0.0025962	6.37E-07	-6.75E-11	2.48E-15	24424.477	-32.254544	34658.816
SnCL2										
0	9524.6659	-432.98456	8.6447203	-0.0034584	4.12E-06	-2.59E-09	6.69E-13	-24329.211	-12.991443	-202648.28
1	-39035.8849	-7.9479627	7.0064876	-2.78E-06	6.46E-10	-7.12E-15	3.69E-18	-26545.297	-3.3680859	-202648.28
SnCL3										
0	17600.76813	-814.28055	13.06327	-0.0063956	7.57E-06	-4.75E-09	1.22E-12	-34134.31	-34.576803	-292372.46
1	-74829.664	-15.285239	10.012403	-5.29E-06	1.23E-09	-1.46E-13	6.97E-18	-38308.783	-16.630637	-292372.46
SnCL4										
0	42459.6787	-1280.5743	17.684453	-0.0095748	1.12E-05	-6.91E-09	1.76E-12	-55040.09	-58.273537	-478465.97
1	-107833.6862	-25.543059	13.020404	-8.60E-06	1.98E-09	-2.34E-13	1.11E-17	-61635.62	-30.727033	-478465.97
SnF										
0	60985.0352	-986.03063	8.9947312	-0.0122301	1.84E-05	-1.27E-08	3.29E-12	-7882.6145	-22.219217	-95017.09
1	25897.15476	-1484.4782	7.3785189	-0.0013242	2.85E-07	-2.36E-11	6.12E-16	-4776.689	-16.812025	-95017.09

SnF2										
0	70423.9185	-1137.506	10.086594	-0.0047229	4.14E-06	-1.92E-09	3.64E-13	-57566.708	-25.715666	-510956.95
1	-102775.8772	-44.517516	7.0332688	-1.33E-05	2.93E-09	-3.36E-13	1.55E-17	-63621.259	-6.8100845	-510956.95
SnF3										
0	109555.5529	-1950.558	15.414078	-0.0085465	7.80E-06	-3.83E-09	7.79E-13	-70567.949	-54.946395	-646630.48
1	-182931.9689	-75.573587	10.056715	-2.28E-05	5.03E-09	-5.78E-13	2.68E-17	-80918.976	-21.91674	-646630.48
SnF4										
0	139044.1119	-2168.7844	16.918029	-0.0023186	-2.05E-06	3.43E-09	-1.29E-12	-115356.34	-63.706048	-1024766.7
1	-263569.2764	-144.547	13.106907	-4.24E-05	9.29E-09	-1.06E-12	4.87E-17	-127154	-38.039219	-1024766.7
SnI										
0	26702.12235	-500.60264	7.4906732	-0.0087463	1.29E-05	-8.21E-09	1.94E-12	21772.492	-9.3548069	172725.02
1	-55549.9185	-1530.4575	7.9326014	-0.0021089	7.81E-07	-1.35E-10	8.21E-15	27448.65	-16.268229	172725.02
SnI2										
0	-5739.25489	-94.350245	7.3779567	-8.26E-04	1.01E-06	-6.51E-10	1.71E-13	-2622.6445	-0.9605815	-8066.737
1	-15594.5339	-1.5947894	7.0013512	-5.94E-07	1.41E-10	-1.70E-14	8.23E-19	-3100.6083	1.2350385	-8066.737
SnI3										
0	-10699.78099	-138.76935	10.556376	-0.0012164	1.49E-06	-9.59E-10	2.52E-13	-3314.2299	-12.495582	-8017.54
1	-25175.3487	-2.3482829	10.001991	-8.75E-07	2.08E-10	-2.51E-14	1.22E-18	-4017.0556	-9.2639085	-8017.54
SnI4										
0	-12831.46793	-145.98851	13.586349	-0.0012836	1.57E-06	-1.01E-09	2.66E-13	-17511.78	-23.679732	-118854.04
1	-28018.40706	-2.4746994	13.002102	-9.25E-07	2.20E-10	-2.66E-14	1.29E-18	-18250.838	-20.274843	-118854.04
SnO										
0	25477.88022	-229.35831	3.4215935	0.0047133	-7.37E-06	5.38E-09	-1.52E-12	2853.0477	6.6739653	21911.054
1	-2555955.548	7870.0535	-5.4397687	0.0063078	-2.07E-06	3.31E-10	-1.85E-14	-48416.639	71.759525	21911.054
SnO2										
0	47076.7408	-611.45687	6.1174339	0.007514	-1.24E-05	9.22E-09	-2.63E-12	2981.0681	-8.1449264	11680.18
1	-157355.8926	-142.73168	7.6057008	-4.20E-05	9.22E-09	-1.05E-12	4.85E-17	-523.45319	-14.283602	11680.18
SnS										
0	27248.77813	-492.41264	6.2216547	-0.0034094	3.98E-06	-2.47E-09	6.34E-13	14524.953	-6.7912753	111099.01
1	-1797985.129	6141.7363	-4.0195049	0.0059938	-2.19E-06	3.90E-10	-2.41E-14	-26113.498	62.568217	111099.01
SnS2										
0	38771.4541	-848.69539	10.42084	-0.0056869	6.37E-06	-3.83E-09	9.50E-13	20060.28	-27.237231	149645.6
1	-67640.8405	-19.701897	7.5153339	-6.33E-06	1.43E-09	-1.68E-13	7.89E-18	15650.536	-9.9227284	149645.6
Sn2										
0	-132966.6654	1639.1798	-1.902869	0.0129043	-1.12E-05	4.50E-09	-6.06E-13	40974.527	44.35408	421343.74
1	-4275783.04	12364.217	-8.4383362	0.0070881	-1.71E-06	1.81E-10	-7.06E-15	-30014.187	100.51385	421343.74
Sr										
0	4.19064984	-0.0630444	2.500373	-1.12E-06	1.79E-09	-1.46E-12	4.75E-16	18558.526	5.5557728	160500
1	1.49E+07	-43753.351	51.372663	-0.0259257	6.58E-06	-6.95E-10	2.42E-14	297754.55	-345.48908	160500
2	5.56E+08	-609319.32	210.90968	-0.0301006	2.18E-06	-7.82E-11	1.11E-15	4579268.3	-1752.7169	160500
Sr+										
0	11.27287678	-0.1346952	2.5006515	-1.64E-06	2.25E-09	-1.61E-12	4.70E-16	85389.812	6.2472592	716166.33
1	3145095.058	-9514.7569	13.500869	-0.0060597	1.59E-06	-1.72E-10	6.32E-15	145799.19	-72.364169	716166.33
2	9.02E+08	-624464.17	169.57636	-0.0215484	1.46E-06	-4.93E-11	6.51E-16	4966238.9	-1431.8446	716166.33
SrBr										
0	-754.9771	-73.59528	4.8280303	-7.16E-04	1.03E-06	-6.89E-10	1.88E-13	-8686.1685	4.1511466	-63917.691
1	3009971.95	-9193.1799	15.260318	-0.0060092	1.69E-06	-2.04E-10	8.81E-15	49227.983	-70.682445	-63917.691
2	2.27E+08	-156599.66	42.345793	-0.0034771	1.36E-07	-2.62E-12	1.97E-17	1221439.3	-326.58246	-63917.691
SrBr2										
0	-4632.45866	-72.449386	7.8002172	-6.77E-04	8.54E-07	-5.63E-10	1.51E-13	-50822.383	-5.2850748	-406725.85
1	-11861.73059	-1.404383	7.5012156	-5.42E-07	1.30E-10	-1.58E-14	7.68E-19	-51185.752	-3.5520371	-406725.85
SrCL										
0	3555.35271	-172.93851	5.2134456	-0.0015429	2.03E-06	-1.33E-09	3.55E-13	-15882.881	0.4818058	-127867.89
1	2070218.603	-6199.8937	11.503146	-0.0036757	9.46E-07	-9.20E-11	2.71E-15	22714.731	-45.6106	-127867.89
2	1.38E+08	-96595.798	26.004308	-0.0014052	2.01E-08	7.12E-13	-2.00E-17	744802.38	-187.68599	-127867.89
SrCL+										
0	1689.043529	-174.92847	5.0653286	-9.86E-04	1.07E-06	-5.99E-10	1.40E-13	48611.903	0.2491965	408112.16
1	-21324.75783	-4.0579483	4.5031494	3.83E-05	2.68E-09	5.67E-14	1.61E-18	47693.26	3.6377188	408112.16
2	-10413.13813	-7.2083024	4.5015898	3.94E-05	2.39E-09	9.06E-14	4.72E-21	47723.575	3.6473717	408112.16
SrCL2										
0	1913.170011	-268.1157	8.0813343	-0.0023933	2.98E-06	-1.94E-09	5.17E-13	-59101.119	-8.4578332	-484813.9
1	-25927.16099	-5.2637859	7.0044752	-1.97E-06	4.68E-10	-5.67E-14	2.74E-18	-60453.995	-2.1922085	-484813.9
SrF										
0	27250.04888	-485.00133	6.1126895	-0.0030085	3.37E-06	-1.99E-09	4.88E-13	-35368.907	-6.6837292	-303552.8
1	870231.859	-2589.8128	7.2002529	-0.0011734	2.00E-07	1.10E-11	-2.34E-15	-21336.755	-16.673864	-303552.8
2	-3.45E+07	22080.505	-5.1257	0.0022091	-1.55E-07	5.13E-12	-6.68E-17	-204858.76	79.955642	-303552.8
SrF+										
0	40096.242	-594.49461	6.1823303	-0.0027162	2.64E-06	-1.38E-09	3.05E-13	26971.494	-8.3136595	209468.31
1	-47520.8206	-25.268023	4.5192953	2.56E-05	3.38E-09	-1.51E-13	9.54E-18	23838.614	1.8921973	209468.31
2	-2403.608095	-32.425687	4.5071248	3.26E-05	1.67E-09	5.13E-14	2.10E-20	23926.92	1.9745171	209468.31
SrF2										
0	41707.5965	-850.01324	10.028061	-0.0060985	7.06E-06	-4.36E-09	1.11E-12	-92178.599	-23.251001	-784793.8
1	-61262.6543	-19.640608	7.0155578	-6.51E-06	1.49E-09	-1.76E-13	8.32E-18	-96567.013	-5.4023088	-784793.8
SrH										
0	-43177.9689	767.64297	-1.5943986	0.0150071	-1.83E-05	1.14E-08	-2.86E-12	21796.857	33.246742	219227.11
1	-226982.5428	1345.2095	1.1521944	0.0031096	-1.19E-06	2.07E-10	-1.30E-14	17355.471	21.129169	219227.11
SrI										
0	-2467.498501	-25.354958	4.6032985	-1.61E-04	2.69E-07	-1.56E-10	3.83E-14	-2175.5383	6.4114819	-7851.676
1	2201136.857	-7082.2307	13.325979	-0.0053059	1.64E-06	-2.21E-10	1.08E-14	42190.772	-55.308332	-7851.676
2	1.56E+08	-115078.77	35.505208	-0.0033753	1.70E-07	-4.44E-12	4.85E-17	891735.79	-261.39173	-7851.676
SrI2										
0	-4391.84969	-37.572674	7.6569935	-3.56E-04	4.51E-07	-2.98E-10	8.02E-14	-35533.035	-2.5982816	-278218.84

1	-8090.38192	-0.7348263	7.5006401	-2.86E-07	6.88E-11	-8.40E-15	4.09E-19	-35721.064	-1.6931191	-278218.84
SrO										
0	42248.9167	-591.35179	5.964363	-0.0021057	2.03E-06	-1.20E-09	3.47E-13	101.80537	-7.5114275	-14207.691
1	-5.17E+07	151082.1	-161.45135	0.0851605	-2.09E-05	2.45E-09	-1.11E-13	-968782.95	1197.847	-14207.691
2	1.99E+08	-94387.337	28.62378	-0.0029233	1.81E-07	-5.72E-12	7.32E-17	758324.63	-203.37026	-14207.691
SrO+										
0	46186.7416	-460.45609	5.6053607	-0.0015117	1.33E-06	-6.24E-10	1.27E-13	76941.405	-3.3774414	630053.72
1	1035147.885	-3339.0811	8.5200553	-0.0023408	7.34E-07	-1.03E-10	5.09E-15	95407.491	-24.912234	630053.72
2	-6.91E+07	12536.862	9.5221594	-0.0012793	9.00E-08	-2.93E-12	3.75E-17	-57785.069	-32.319588	630053.72
SrOH										
0	46400.0656	-993.86855	9.784949	-0.0057744	5.13E-06	-1.83E-09	1.93E-13	-20227.212	-27.40671	-194085.73
1	2545648.379	-7416.196	13.819562	-0.0030965	7.72E-07	-7.92E-11	2.74E-15	22313.021	-61.487811	-194085.73
SrOH+										
0	38573.6694	-903.02423	9.4511033	-0.0050425	4.19E-06	-1.20E-09	1.61E-14	39950.677	-26.014861	310169.61
1	867969.566	-2340.6095	7.9768298	1.02E-04	-6.29E-08	1.02E-11	-5.72E-16	50731.577	-20.270469	310169.61
Sr(OH)2										
0	72050.903	-1789.4652	17.294291	-0.0116928	1.11E-05	-4.49E-09	6.60E-13	-66053.94	-63.886812	-596694.57
1	1750013.518	-4681.6015	13.955484	2.04E-04	-1.25E-07	2.04E-11	-1.14E-15	-44271.702	-50.514569	-596694.57
SrS										
0	12564.40807	-315.04366	5.7217225	-0.0026305	3.38E-06	-2.30E-09	6.51E-13	12772.952	-3.6938624	104351.32
1	-1.38E+07	39213.316	-36.028664	0.0181851	-3.28E-06	2.32E-10	-3.61E-15	-241024.62	299.16798	104351.32
Sr2										
0	-110885.9753	592.7604	8.4396886	-0.026528	4.44E-05	-3.40E-08	9.97E-12	31576.15	-7.0339667	307570.34
1	209844.5682	103.86501	2.3093323	1.33E-04	-4.43E-08	6.71E-12	-3.37E-16	36366.427	21.680885	307570.34
Ta										
0	-11509.07339	47.807304	3.1855884	-0.0053665	1.29E-05	-1.05E-08	3.05E-12	92997.976	5.3360566	782518.64
1	1689726.898	-5986.8547	9.5650397	-0.0025116	6.44E-07	-7.19E-11	3.11E-15	130671.1	-43.350963	782518.64
2	-8.41E+08	638150.9	-185.60319	0.0279735	-2.07E-06	7.40E-11	-1.02E-15	-4836410.6	1607.0078	782518.64
Ta+										
0	286971.2865	-3084.921	14.306797	-0.0198477	1.95E-05	-8.97E-09	1.50E-12	201382.87	-63.064278	1549679.3
1	3656142.13	-12540.735	18.650226	-0.0079433	2.15E-06	-2.82E-10	1.41E-14	263687.65	-106.58643	1549679.3
2	3.72E+07	-34057.093	16.300563	-0.002065	1.62E-07	-5.75E-12	7.64E-17	440511.55	-104.02377	1549679.3
Ta-										
0	187398.2301	-1681.2687	6.4800402	-2.25E-04	2.03E-06	-4.68E-09	2.00E-12	97934.96	-20.496182	745469.43
1	-4235467.48	11010.564	-4.7369111	0.0025036	-4.82E-07	4.89E-11	-2.03E-15	15746.994	64.918027	745469.43
2	414988.403	1227.9721	2.2092116	3.40E-05	-2.14E-09	6.91E-14	-9.02E-19	82490.656	11.956362	745469.43
TaCL5										
0	63064.8329	-1771.2214	22.550834	-0.0136024	1.61E-05	-1.02E-08	2.63E-12	-87927.371	-80.978649	-764835
1	-142644.4545	-38.943403	16.031424	-1.33E-05	3.08E-09	-3.66E-13	1.75E-17	-97012.972	-42.56987	-764835
TaO										
0	0	0	2.9340108	0.0030592	-1.94E-06	1.63E-10	3.02E-13	22154.472	11.454646	192468.83
1	0	0	3.4996603	0.0015113	-6.54E-07	1.78E-10	-1.69E-14	21994.151	8.526959	192468.83
TaO2										
0	0	0	3.1803826	0.0094703	-8.73E-06	2.45E-09	3.37E-13	-25451.762	13.130353	-200835.09
1	0	0	5.9701669	0.0011792	-5.65E-07	1.31E-10	-1.06E-14	-26169.481	-1.073998	-200835.09
Ti										
0	-45701.794	660.8092	0.4295257	0.003615	-3.55E-06	1.76E-09	-3.05E-13	52709.479	20.261497	473000
1	-170478.6714	1073.8528	1.181955	2.25E-04	3.09E-07	-5.74E-11	2.93E-15	49780.699	17.404314	473000
2	1.15E+09	-722240.84	177.71675	-0.0200806	1.22E-06	-3.81E-11	4.80E-16	5772614.5	-1518.0805	473000
Ti+										
0	170745.7044	-1727.5246	9.6158853	-0.0108966	8.20E-06	-2.87E-09	3.42E-13	144789.76	-34.631437	1137624
1	-768546.308	2545.8681	0.3423863	7.10E-04	2.71E-08	-2.37E-11	1.90E-15	119882.15	24.847992	1137624
2	3.92E+07	-25345.816	9.5867597	-7.58E-04	4.43E-08	-8.44E-13	-4.52E-19	334444.06	-52.200263	1137624
Ti-										
0	-3006.48499	204.09117	1.822639	0.0012453	-1.31E-06	7.37E-10	-1.72E-13	53467.721	12.059266	459203.81
1	23411.1764	2.5804139	2.4977546	9.77E-07	-2.28E-10	2.72E-14	-1.30E-18	54546.622	7.999824	459203.81
2	14175.14172	5.6387996	2.4987517	1.43E-07	-8.89E-12	2.87E-16	-3.75E-21	54518.435	7.9941095	459203.81
TiCL										
0	0	0	2.8543089	0.0079593	-9.82E-06	5.24E-09	-9.80E-13	17441.216	11.729991	154393.16
1	0	0	5.296976	-1.64E-04	1.57E-07	-3.86E-11	3.07E-15	16857.674	-0.4947067	154393.16
TiCL2										
0	0	0	4.9723475	0.0112773	-2.06E-05	1.72E-08	-5.40E-12	-30366.285	2.5589322	-237237.62
1	0	0	7.7624852	-9.39E-04	8.01E-07	-1.90E-10	1.50E-14	-30915.805	-10.752765	-237237.62
TiCL3										
0	0	0	2.8801557	0.0335589	-6.00E-05	4.89E-08	-1.51E-11	-66776.023	13.958082	-539328.97
1	0	0	10.008103	4.19E-04	-2.15E-07	4.53E-11	-3.45E-15	-68061.25	-19.51078	-539328.97
TiCL4										
0	0	0	6.9496757	0.0260497	-4.65E-05	3.84E-08	-1.20E-11	-94677.831	-2.9258537	-763178.78
1	0	0	12.38603	7.09E-04	-3.17E-07	6.26E-11	-4.53E-15	-95669.078	-28.471698	-763178.78
TiO										
0	0	0	3.1198881	0.0031202	-1.33E-06	-1.33E-09	9.63E-13	5486.8719	9.4423067	54392.051
1	0	0	4.1360176	7.39E-04	-4.54E-07	1.30E-10	-1.15E-14	5198.3483	4.1220651	54392.051
TiOCL										
0	0	0	3.4093856	0.0151706	-2.44E-05	1.87E-08	-5.57E-12	-30887.846	8.6942299	-244267.7
1	0	0	6.8319924	7.64E-04	-3.40E-07	6.67E-11	-4.81E-15	-31582.311	-7.7540125	-244267.7
TiOCL2										
0	0	0	5.440814	0.017705	-2.95E-05	2.32E-08	-7.05E-12	-67806.854	3.4506286	-545564.73
1	0	0	9.3368655	7.60E-04	-3.38E-07	6.65E-11	-4.80E-15	-68572.645	-15.144322	-545564.73
TiO2										
0	0	0	3.0142717	0.0109421	-1.29E-05	7.12E-09	-1.49E-12	-38020.501	11.364153	-305440.77
1	0	0	5.8455061	0.0013938	-6.64E-07	1.39E-10	-9.88E-15	-38700.593	-2.7962432	-305440.77
V										

0	-55353.7602	559.33385	2.6755435	-0.006243	1.57E-05	-1.37E-08	4.17E-12	58206.644	9.5245675	517267.06
1	1200390.3	-5027.0053	10.588306	-0.0050443	1.49E-06	-1.79E-10	8.11E-15	91707.409	-47.683363	517267.06
2	2.46E+09	-1339992	278.10399	-0.0263894	1.30E-06	-3.21E-11	3.10E-16	1.09E+07	-2439.9544	517267.06
V+										
0	75688.3446	-841.52738	7.5592327	-0.0144172	2.04E-05	-1.29E-08	3.07E-12	144447.82	-19.910676	1173745.4
1	2347072.054	-9021.1972	14.773498	-0.0068919	1.97E-06	-2.54E-10	1.23E-14	195835.14	-78.555929	1173745.4
2	2.52E+08	-186647.67	56.335871	-0.0071985	5.07E-07	-1.70E-11	2.16E-16	1585980.5	-451.28226	1173745.4
V-										
0	-3799.27356	231.38404	1.7256082	0.0014293	-1.51E-06	8.49E-10	-1.99E-13	53474.029	12.61901	460386.06
1	26001.0043	2.0963341	2.4980065	8.99E-07	-2.14E-10	2.58E-14	-1.24E-18	54700.071	7.9779002	460386.06
2	16011.0291	5.8209749	2.4987055	1.48E-07	-9.27E-12	3.00E-16	-3.92E-21	54666.926	7.9745574	460386.06
VCL4										
0	0	0	7.1166462	0.0254232	-4.55E-05	3.76E-08	-1.18E-11	-66123.893	-2.3309548	-525521.53
1	0	0	12.718647	1.66E-05	1.42E-07	-3.48E-11	2.29E-15	-67187.992	-28.84801	-525521.53
VN										
0	0	0	2.723359	0.0041643	-2.19E-06	-1.24E-09	1.08E-12	61927.893	11.417358	523013.12
1	0	0	4.185228	6.15E-04	-3.58E-07	1.07E-10	-9.73E-15	61511.54	3.7761866	523013.12
VO										
0	0	0	2.9438441	0.0029059	-9.95E-07	-1.41E-09	9.24E-13	14352.746	10.186431	127615.03
1	0	0	3.9114702	7.75E-04	-4.23E-07	1.16E-10	-1.01E-14	14065.204	5.0718541	127615.03
VO2										
0	0	0	3.1937859	0.0092979	-8.34E-06	2.10E-09	4.46E-13	-29275.491	11.287219	-232634.44
1	0	0	5.9470147	0.0011687	-5.05E-07	9.67E-11	-6.82E-15	-29983.802	-2.7380251	-232634.44
W										
0	159522.3922	-2673.8439	20.604697	-0.0625232	1.11E-04	-8.45E-08	2.34E-11	113964.86	-90.118369	851243.53
1	-8048745.96	14657.004	-0.2508532	-0.0025965	1.41E-06	-2.23E-10	1.26E-14	-3091.1309	39.558222	851243.53
2	1.42E+09	-432536.56	-8.8416151	0.0164554	-1.91E-06	8.53E-11	-1.36E-15	3994798.8	-12.664182	851243.53
W+										
0	-196928.4929	2670.1373	-11.316869	0.0330818	-3.63E-05	2.07E-08	-4.81E-12	182095.09	85.521045	1627841
1	6387743.4	-20618.115	27.592916	-0.0124454	3.27E-06	-4.07E-10	1.91E-14	324517.44	-171.69192	1627841
2	6.84E+07	-89817.118	38.457208	-0.0054658	4.02E-07	-1.34E-11	1.67E-16	854693.28	-289.28055	1627841
W-										
0	0	0	2.5	0	0	0	0	91429.814	8.4611697	766391.53
1	0	0	2.5	0	0	0	0	91429.814	8.4611697	766391.53
2	0	0	2.5	0	0	0	0	91429.814	8.4611697	766391.53
WCL6										
0	33393.9167	-1697.3661	25.606124	-0.0142525	1.74E-05	-1.12E-08	2.95E-12	-56730.592	-97.41467	-493712
1	-151673.5473	-34.513793	19.028672	-1.24E-05	2.92E-09	-3.51E-13	1.69E-17	-65357.798	-58.949156	-493712
WOCL4										
0	26588.12693	-933.69132	13.213774	0.0127093	-1.96E-05	1.41E-08	-3.90E-12	-67922.908	-35.948702	-573493
1	-304902.8285	-353.94259	16.264327	-1.06E-04	2.34E-08	-2.69E-12	1.25E-16	-72725.467	-49.917618	-573493
WO2										
0	3120.918919	241.38835	-0.3024119	0.0232433	-3.38E-05	2.38E-08	-6.42E-12	1442.0053	29.576552	29061.744
1	-753740.668	3204.6431	0.6701966	0.0044882	-8.86E-07	6.25E-11	-9.05E-16	-17694.202	34.05724	29061.744
WO2CL2										
0	430.015448	-243.85479	7.976307	0.0171501	-2.49E-05	1.74E-08	-4.77E-12	-82328.124	-7.8447746	-671532
1	-240479.173	-306.83796	13.228145	-9.10E-05	2.01E-08	-2.30E-12	1.06E-16	-83674.931	-34.915569	-671532
WO3										
0	7262.46146	34.293911	1.573062	0.0275497	-3.99E-05	2.81E-08	-7.78E-12	-40017.333	18.5741	-319725.21
1	1732203.64	-6284.7198	16.813589	-0.0034721	8.08E-07	-6.59E-11	1.14E-15	-2473.0756	-74.074741	-319725.21
WO3-										
0	163099.9684	-1967.6097	12.019709	0.0016813	-5.86E-06	5.03E-09	-1.43E-12	-70092.04	-39.36901	-650475.96
1	463783.251	-1347.0893	9.7736376	0.0010714	-3.84E-07	5.74E-11	-3.16E-15	-72395.156	-23.911163	-650475.96
(WO3)2										
0	80884.1451	-906.03408	7.6015754	0.0524101	-7.92E-05	5.71E-08	-1.61E-11	-144149.7	-10.935241	-1210443.3
1	-667407.243	-703.25184	22.516175	-2.04E-04	4.44E-08	-5.05E-12	2.32E-16	-150269.95	-86.13989	-1210443.3
(WO3)3										
0	34853.9001	-193.34963	8.2065448	0.0859952	-1.26E-04	8.89E-08	-2.47E-11	-246245.35	-5.6573253	-2013291.1
1	-945026.331	-1133.8372	34.834792	-3.30E-04	7.23E-08	-8.22E-12	3.79E-16	-248848.63	-144.15511	-2013291.1
(WO3)4										
0	13886.06167	228.75186	8.66237	0.1219701	-1.77E-04	1.25E-07	-3.46E-11	-346783.96	-3.6039373	-2817433.9
1	-1277530.217	-1566.5385	47.153635	-4.56E-04	9.99E-08	-1.14E-11	5.23E-16	-347741.85	-205.15884	-2817433.9
(WO3)5										
0	14975.76743	271.99998	11.386269	0.1523302	-2.21E-04	1.56E-07	-4.32E-11	-437142.43	-14.416435	-3551492.3
1	-1600667.953	-1958.4379	59.442274	-5.71E-04	1.25E-07	-1.42E-11	6.54E-16	-438409.59	-266.02388	-3551492.3
Xe										
0	0	0	2.5	0	0	0	0	-745.375	6.1644199	0
1	4025.22668	-12.095075	2.5141533	-8.25E-06	2.53E-09	-3.89E-13	2.36E-17	-668.58007	6.0636764	0
2	2.54E+08	-110537.38	13.826441	0.0015006	-3.94E-07	2.77E-11	-5.94E-16	928544.38	-110.98349	0
Xe+										
0	100.292362	-1.2187536	2.5060165	-1.55E-05	2.19E-08	-1.62E-11	4.93E-15	140766.54	7.5166782	1176552.2
1	-12416.83887	-150.06546	2.9646783	-4.69E-04	1.96E-07	-3.04E-11	1.64E-15	141496.68	4.5656515	1176552.2
2	-2.56E+08	157047.69	-36.355372	0.0050194	-3.44E-07	1.14E-11	-1.30E-16	-1103556.5	343.61885	1176552.2
Zn										
0	0	0	2.5	0	0	0	0	14938.051	5.118861	130400
1	-175559.1489	498.41392	1.9693863	2.61E-04	-5.63E-08	2.72E-12	4.27E-16	11737.735	8.9610857	130400
2	-2.09E+08	157817.81	-36.220331	0.0033452	-8.57E-09	-7.12E-12	1.69E-16	-1217847.7	345.944	130400
Zn+										
0	4.10E-04	-4.34E-06	2.5	-4.39E-11	5.56E-14	-3.64E-17	9.61E-21	124697.99	5.8119955	1043000.1
1	-343617.946	956.73552	1.511479	4.61E-04	-8.79E-08	7.56E-13	1.17E-15	118532.19	13.007427	1043000.1
2	-3.01E+09	2074729.3	-558.9527	0.075014	-5.14E-06	1.74E-10	-2.32E-15	-1.61E+07	4824.788	1043000.1
Zr										

0	67158.9996	-943.59817	6.3597562	-9.79E-04	-7.61E-06	9.31E-09	-3.12E-12	75880.195	-16.657705	599318.61
1	6006771.84	-15669.606	17.969824	-0.0067634	1.73E-06	-2.06E-10	9.33E-15	173463.62	-105.11174	599318.61
2	5.21E+08	-282565.24	60.770544	-0.0050812	2.35E-07	-6.24E-12	8.01E-17	2351487.4	-509.31831	599318.61
Zr+										
0	173984.2193	-2224.5985	14.007878	-0.0237879	2.64E-05	-1.44E-08	3.14E-12	159821.07	-58.167288	1246246.3
1	729813.716	-2017.1176	5.0374983	-5.50E-04	1.02E-07	-1.26E-11	7.09E-16	162088.49	-9.8206409	1246246.3
2	-2.29E+07	18609.727	-1.66151	6.02E-04	-3.93E-08	1.54E-12	-2.62E-17	4907.2989	46.421305	1246246.3
Zr-										
0	30466.62367	-807.42772	9.2130061	-0.0161434	1.91E-05	-1.14E-08	2.75E-12	69030.34	-28.626444	552952.4
1	84718.6116	317.54393	2.2514912	1.02E-04	-2.29E-08	2.65E-12	-1.24E-16	64223.376	10.812611	552952.4
2	-438664.156	376.87487	2.4170884	9.41E-06	-5.82E-10	1.87E-14	-2.42E-19	63347.011	9.6777787	552952.4
ZrN										
0	0	0	3.0718872	0.002643	3.18E-07	-3.63E-09	2.03E-12	84768.495	9.8058899	713372
1	0	0	4.1437892	4.04E-04	-1.45E-07	2.48E-11	-1.54E-15	84461.42	4.1593791	713372
ZrO										
0	-509176.14	8652.7701	-52.947402	0.1728962	-2.46E-04	1.67E-07	-4.42E-11	-30951.298	313.25767	83922.708
1	464809.831	344.23145	4.8157792	-4.66E-04	2.14E-07	-2.05E-11	4.08E-16	7317.3407	1.5029335	83922.708
2	1.34E+08	-78510.884	19.816142	-8.03E-04	2.52E-09	7.96E-13	-1.68E-17	640667.06	-135.84723	83922.708
ZrO+										
0	10329.11549	73.046612	2.6063453	0.0050993	-6.25E-06	3.80E-09	-9.20E-13	85332.338	12.67311	720614.11
1	-493716.656	669.99008	4.5753535	-6.92E-04	4.28E-07	-7.55E-11	4.41E-15	80188.807	2.9289437	720614.11
2	4.39E+07	-20840.442	8.1671262	-5.67E-05	-8.86E-09	4.77E-13	-7.44E-18	255451.79	-31.271524	720614.11
ZrO2										
0	0	0	3.2103779	0.011629	-1.56E-05	1.00E-08	-2.54E-12	-35775.612	11.773868	-286189.8
1	0	0	6.1418545	9.77E-04	-4.33E-07	8.50E-11	-6.13E-15	-36446.178	-2.7097891	-286189.8
Ag(cr)										
0	-70992.3647	725.4788	0.1066518	0.0055295	-4.43E-06	2.09E-09	-3.89E-13	-4614.0143	5.074216	0
Ag(L)										
0	0	0	4.0170738	0	0	0	0	-467.227	-17.715271	0
AL(cr)										
0	-62518.1143	634.39344	-0.7131884	0.0108873	-1.46E-05	9.96E-09	-1.77E-12	-3985.4393	6.5611002	0
AL(L)										
0	0	0	3.8186255	0	0	0	0	-95.763232	-17.525534	0
ALBr3(cr)										
0	-190729.2099	0	26.656627	-0.083261	1.40E-04	0	0	-67638.811	-112.65227	-511500
ALBr3(L)										
0	0	0	15.033959	0	0	0	0	-64814.021	-60.836177	-511500
ALCL3(cr)										
0	-260555.1108	2535.7624	-1.2483791	0.0246543	-8.05E-06	0	0	-100777.7	20.303757	-705100
ALCL3(L)										
0	0	0	15.094095	0	0	0	0	-85590.225	-65.190146	-705100
ALF3(II)										
0	0	0	-2.4446212	0.0624861	-8.04E-05	0	0	-182996.12	6.8715852	-1510400
1	0	0	-3.1585746	0.0710137	-1.25E-04	7.93E-08	0	-182928.33	9.6614694	-1510400
ALF3(I)										
0	-106067.5855	0	11.140524	0.0010927	0	0	0	-185350.22	-56.51122	-1510400
ALH3(a)										
0	574461.299	-7649.5797	34.813554	-0.0449574	2.95E-05	0	0	35497.932	-205.07276	-11400
ALI3(cr)										
0	-3486.28046	0	8.6443744	0.0108807	5.04E-07	0	0	-39507.364	-29.686619	-302900
ALI3(L)										
0	0	0	14.552872	0	0	0	0	-39139.032	-56.704888	-302900
ALN(cr)										
0	3654.74153	0	-2.1486005	0.0274444	-2.76E-05	0	0	-38689.483	7.7339692	-319000
1	-180154.934	0	5.5252805	4.03E-04	0	0	0	-40636.165	-30.188299	-319000
ALN(L)										
0	0	0	4.4911847	9.46E-04	0	0	0	-39555.189	-23.387703	-319000
1	0	0	8.0582019	0	0	0	0	-37559.284	-45.987313	-319000
AL(OH)3(a)										
0	-23767.48819	928.97912	-15.323373	0.1307578	-2.21E-04	1.57E-07	0	-160548.58	67.95129	-1293500
AL2O3(a)										
0	-5391549.97	103667.7	-817.32292	3.3882587	-0.0075124	8.66E-06	-4.07E-09	-666013.47	4235.5022	-1675700
1	-604208.7868	0	14.754808	8.27E-04	0	0	0	-207923.54	-81.360295	-1675700
2	0	0	12.937744	0.0019928	0	0	0	-206078.76	-69.666037	-1675700
AL2O3(L)										
0	0	0	19.592255	0	0	0	0	-202770.16	-110.8591	-1675700
AL2S3(a)										
0	0	0	-1.3478101	0.0847815	-1.27E-04	0	0	-80240.147	2.1036446	-648500
1	-194310.9095	0	14.176181	0.0021649	0	0	0	-82970.75	-68.453621	-648500
AL2S3(b)										
0	0	0	16.838034	0	0	0	0	-84452.515	-84.667698	-648500
AL2S3(L)										
0	0	0	19.243467	0	0	0	0	-81140.233	-97.228486	-648500
AL2SiO5(an)										
0	0	0	-9.2866342	0.1347672	-2.32E-04	1.88E-07	-5.74E-11	-313276.64	32.715859	-2592171.4
1	0	0	17.351742	0.0087438	-3.71E-06	1.07E-09	-1.18E-13	-317941.51	-91.738744	-2592171.4
AL4C3(cr)										
0	4384.12758	0	-5.8037797	0.1009596	-1.16E-04	0	0	-26602.637	18.84004	-206900
1	-448360.7573	0	17.889208	0.0040243	0	0	0	-31900.563	-94.949107	-206900
AL6Si2O13(s)										
0	0	0	-11.034671	0.2667564	-4.15E-04	3.14E-07	-9.25E-11	-825658.7	32.254791	-6819432.1
1	0	0	45.238364	0.0276614	-1.47E-05	3.89E-09	-3.67E-13	-836864.17	-237.39565	-6819432.1

B(b)										
0	259825.9342	-4770.7731	34.641245	-0.1287342	2.90E-04	-3.31E-07	1.50E-10	21469.468	-183.08247	0
1	-869.770022	-805.0406	4.0797129	-6.42E-04	4.85E-07	-1.25E-10	1.34E-14	3397.9199	-25.059066	0
B(L)										
0	0	0	3.8186255	0	0	0	0	3360.6031	-20.731673	0
BN(cr)										
0	492731.243	-6086.4069	26.782268	-0.0452969	5.31E-05	-3.04E-08	6.80E-12	-241.34749	-157.0534	-251000
1	-839403.949	0	6.2312566	-1.26E-05	2.02E-09	0	0	-34272.692	-36.872609	-251000
BN(L)										
0	0	0	8.0582019	0	0	0	0	-30234.1	-48.623824	-251000
B2O3(cr)										
0	-55952.9738	1311.2142	-11.785359	0.077028	-9.74E-05	4.69E-08	1.80E-12	-159967.29	58.667592	-1273500
B2O3(L)										
0	377412.4994	0	15.280155	0	0	0	0	-156211.58	-80.560949	-1273500
B2S3(cr)										
0	-94305.01617	0	11.900882	0.0087113	0	0	0	-33477.752	-58.906964	-243000
B2S3(L)										
0	0	0	17.559664	0	0	0	0	-29212.346	-82.681261	-243000
B3O3H3(cr)										
0	0	0	8.1595137	-0.0070668	9.25E-05	-1.03E-07	3.50E-11	-154569.63	-27.525404	-1262313
1	0	0	-12.847052	0.0919581	-8.11E-05	3.27E-08	-5.02E-12	-151109.72	70.153615	-1262313
B4C(cr)										
0	-3.58E+07	674888.41	-5160.6301	20.499735	-0.0445365	5.05E-05	-2.34E-08	-3040618.1	26936.175	-62000
1	-577290.497	0	12.743734	5.72E-05	1.29E-06	0	0	-13206.218	-72.669625	-62000
B4C(cr)										
0	-3.58E+07	674888.41	-5160.6301	20.499735	-0.0445365	5.05E-05	-2.34E-08	-3040618.1	26936.175	-62000
1	-577290.497	0	12.743734	5.72E-05	1.29E-06	0	0	-13206.218	-72.669625	-62000
Ba(cr)										
0	-1121.41305	0	2.7940312	0.0030898	-8.81E-06	1.74E-08	0	-930.6838	-9.1097871	0
1	0	0	2.7733444	0.0020375	0	0	0	-917.43381	-8.9097063	0
Ba(L)										
0	0	0	4.8108668	0	0	0	0	-992.06238	-20.002757	0
BaBr2(cr)										
0	-7817.658527	0	8.4330887	0.0026449	0	0	0	-93102.398	-30.840135	-752000
BaBr2(L)										
0	0	0	12.628525	0	0	0	0	-92274.943	-53.914939	-752000
BaCO3(a)										
0	-2.88E+07	541351.05	-4125.2976	16.386201	-0.0355819	4.03E-05	-1.87E-08	-2581769.9	21548.269	-1214000
1	-457826.1377	0	18.976223	-0.0161417	1.49E-05	0	0	-152617.68	-93.063897	-1214000
BaCO3(b)										
0	0	0	19.002924	0	0	0	0	-153404.29	-99.965682	-1214000
BaCO3(c)										
0	0	0	19.243467	0	0	0	0	-153352.1	-101.3948	-1214000
BaCO3(L)										
0	0	0	19.844825	0	0	0	0	-149640.51	-103.27982	-1214000
BaCL2(a)										
0	-73764.4412	1806.7608	-14.158376	0.1391572	-4.18E-04	6.21E-07	-3.58E-10	-112727.39	73.499006	-855200
1	709.6028509	0	8.3432457	0.0023007	0	0	0	-105443.44	-33.339897	-855200
BaCL2(b)										
0	0	0	15.755589	0	0	0	0	-110580.33	-81.3788	-855200
BaCL2(L)										
0	0	0	13.109612	0	0	0	0	-105408.88	-60.999877	-855200
BaF2(a)										
0	144169.3954	-4606.2838	54.121804	-0.2221461	5.73E-04	-7.32E-07	3.72E-10	-128375.62	-264.92775	-1206000
1	-21805.25371	0	7.7304616	0.0035877	0	0	0	-147585.46	-33.649249	-1206000
BaF2(b)										
0	0	0	15.15423	0	0	0	0	-153354.83	-81.539428	-1206000
BaF2(c)										
0	0	0	15.515045	0	0	0	0	-153582.14	-83.966079	-1206000
BaF2(L)										
0	0	0	12.628525	0	0	0	0	-146704.52	-61.292403	-1206000
BaI2(cr)										
0	15103.32529	-622.4807	15.450378	-0.0323944	9.25E-05	-1.25E-07	6.80E-11	-73056.296	-63.646962	-606000
1	-324.733508	0	8.6077231	0.0023998	0	0	0	-75558.731	-29.891607	-606000
BaI2(L)										
0	0	0	13.590699	0	0	0	0	-76112.648	-58.631835	-606000
BaH2(a)										
0	0	0	4.5308743	0.0033593	0	0	0	-24351.808	-19.239557	-190000
BaH2(b)										
0	0	0	8.5392885	0	0	0	0	-25895.361	-42.675855	-190000
BaH2(L)										
0	0	0	9.0203752	0	0	0	0	-23597.21	-44.144139	-190000
BaO(cr)										
0	-3734308.68	70304.827	-533.41419	2.1431359	-0.0046642	5.29E-06	-2.46E-09	-383316.33	2789.0476	-548000
1	-75518.58137	0	6.7989575	-0.0012055	7.33E-07	0	0	-68142.164	-30.176185	-548000
2	1.38E+07	0	-16.859923	0.0116625	0	0	0	-37049.06	127.4566	-548000
BaO(L)										
0	0	0	10.01863	0	0	0	0	-68614.303	-52.673268	-548000
Ba(OH)2(b)										
0	50787.178	-1641.9969	19.642785	-0.0373061	1.04E-04	-8.66E-08	2.28E-11	-108558.55	-97.015037	-940600
Ba(OH)2(a)										
0	0	0	14.913687	0	0	0	0	-117611.75	-72.522412	-940600

Ba(OH)2(L)										
0	0	0	16.59749	0	0	0	0	-116834.07	-80.681042	-940600
BaS(cr)										
0	336978.647	-6138.7402	49.225538	-0.1599275	3.31E-04	-3.60E-07	1.61E-10	-30282.49	-253.91252	-470000
1	-20506.31967	0	5.9208528	8.31E-04	0	0	0	-58398.689	-24.662338	-470000
BaS(L)										
0	0	0	8.0582019	0	0	0	0	-53560.755	-36.275777	-470000
BaSO4(a)										
0	-1.71E+07	321278.99	-2441.8201	9.7130679	-0.0210502	2.38E-05	-1.10E-08	-1624344	12760.58	-1470000
1	-274700.4935	0	13.520941	0.0062	0	0	0	-182027.54	-64.543155	-1470000
BaSO4(b)										
0	0	0	20.446184	0	0	0	0	-184209.12	-105.0884	-1470000
BaSO4(L)										
0	0	0	20.446184	0	0	0	0	-179398.25	-102.49214	-1470000
Be(a)										
0	3532.37894	0	-1.827528	0.0189548	-2.12E-05	0	0	-98.321469	6.8668941	0
1	-70647.5788	0	2.5503608	6.85E-04	1.16E-07	0	0	-1028.8037	-13.994715	0
Be(b)										
0	0	0	3.6081501	0	0	0	0	-852.44978	-20.028958	0
Be(L)										
0	0	0	3.5456088	0	0	0	0	207.47558	-18.953413	0
BeAL2O4(s)										
0	0	0	-8.054738	0.1135724	-1.88E-04	1.48E-07	-4.48E-11	-277980.44	27.135719	-2300807.9
1	0	0	20.265559	-0.0104666	2.30E-05	-1.55E-08	3.60E-12	-283363.01	-107.47222	-2300807.9
BeAL2O4(L)										
0	0	0	29.636291	0	0	0	0	-280569.82	-171.16954	0
BeBr2(cr)										
0	-129652.8599	0	9.5445192	8.97E-04	0	0	0	-46377.671	-42.388106	-358000
BeBr2(L)										
0	0	0	12.027167	0	0	0	0	-45712.231	-55.345384	-358000
BeCO3(cr)										
0	-368873.2108	0	10.574285	0.0046701	0	0	0	-130281.4	-57.461097	-1045000
BeCL2(a)										
0	-969633.654	16538.413	-112.03229	0.4343457	-8.23E-04	7.97E-07	-3.09E-10	-137216.72	598.11918	-496200
BeCL2(b)										
0	0	0	8.0569992	0.0025161	0	0	0	-61695.055	-37.015173	-496200
BeCL2(L)										
0	0	0	11.064994	0	0	0	0	-62127.516	-53.423823	-496200
BeF2(a)										
0	308258.2728	-5000.7454	30.490664	-0.0541615	5.85E-05	0	0	-101192.89	-168.79615	-1027000
BeF2(b)										
0	0	0	5.6525279	0.0039869	0	0	0	-125290.3	-26.797001	-1027000
BeF2(L)										
0	-1882035.141	0	12.344684	-1.84E-04	0	0	0	-131098.64	-68.981026	-1027000
BeI2(cr)										
0	-144374.1122	0	10.078285	3.37E-04	0	0	0	-26475.947	-43.781706	-191000
BeI2(L)										
0	0	0	12.027167	0	0	0	0	-25510.704	-53.49838	-191000
BeO(a)										
0	204770.1543	-2981.1732	13.856433	-0.015817	2.35E-05	-1.94E-08	6.52E-12	-59222.192	-82.311137	-609400
1	1024057.237	1937.4656	-2.1702139	0.0067009	-1.83E-06	2.76E-10	-2.71E-14	-82768.09	18.966074	-609400
BeO(b)										
0	0	0	6.7352135	0	0	0	0	-76744.749	-39.375288	-609400
BeO(L)										
0	0	0	10.10282	0	0	0	0	-76002.432	-62.538054	-609400
Be(OH)2(b)										
0	-2.82E+07	530602.62	-4050.1247	16.082857	-0.0349114	3.96E-05	-1.83E-08	-2495097.9	21145.704	-905700
1	-454927.5904	0	11.983629	0.002035	0	0	0	-114119.24	-65.974319	-905700
BeS(cr)										
0	-106115.6941	0	4.876054	0.0013639	0	0	0	-30254.443	-24.696064	-236000
BeSO4(a)										
0	967405.285	-15259.769	90.780193	-0.2151324	3.41E-04	-2.62E-07	8.14E-11	-74170.507	-502.43805	-1200000
BeSO4(b)										
0	0	0	18.04075	0	0	0	0	-150808.53	-96.707193	-1200000
BeSO4(c)										
0	0	0	18.04075	0	0	0	0	-150555.96	-96.430251	-1200000
BeSO4(L)										
0	0	0	18.04075	0	0	0	0	-149834.33	-95.914801	-1200000
Be2C(s)										
0	0	0	4.437417	0.0025695	0	0	0	-15507.324	-24.086121	-116986.03
1	0	0	4.437417	0.0025695	0	0	0	-15507.324	-24.086121	-116986.03
Be2C(L)										
0	0	0	11.070897	0	0	0	0	-14969.641	-65.775116	-116986.03
Be3N2(a)										
0	644334.131	-9239.8809	42.113332	-0.0451333	3.23E-05	0	0	-26749.203	-251.15443	-588000
1	-227846.5381	443.21914	1.3762747	0.0322538	-2.70E-05	8.12E-09	-6.68E-14	-75627.438	-11.976256	-588000
Be3N2(b)										
0	0	0	17.439392	0	0	0	0	-78509.422	-101.63028	-588000
Be3N2(L)										
0	0	0	20.085369	0	0	0	0	-71823.038	-116.95406	-588000
Br2(cr)										
0	1079338.54	-9504.3187	-89.515021	1.6459291	-0.0086332	2.01E-05	-1.74E-08	54824.801	247.69362	0

Br2(L)										
0	4023495.18	-39525.326	-22.469768	1.9584628	-0.0101582	2.16E-05	-1.71E-08	213432.26	-253.26132	0
1	0	0	9.0566864	0	0	0	0	-2699.8556	-33.2935	0
C(gr)										
0	113285.676	-1980.4217	13.653842	-0.046361	1.02E-04	-1.08E-07	4.47E-11	8943.8598	-72.958247	0
1	335600.441	-2596.5284	6.9488419	-0.0034848	1.84E-06	-5.06E-10	5.75E-14	13984.125	-44.77183	0
2	202310.5106	-1138.2359	3.7002795	-1.83E-04	6.34E-08	-7.07E-12	3.34E-16	5848.1349	-23.509253	0
Ca(a)										
0	-838564.472	17652.861	-146.45982	0.6316167	-0.0013292	1.12E-06	0	-78262.847	754.96427	0
1	-626229.648	8185.5658	-40.639867	0.1203864	-1.80E-04	1.44E-07	-4.73E-11	-40643.405	231.53155	0
Ca(b)										
0	0	0	5.7011177	-0.0058106	4.02E-06	0	0	-1516.7391	-26.075719	0
Ca(L)										
0	0	0	4.5703235	0	0	0	0	-982.21881	-21.19877	0
CaBr2(cr)										
0	-28263.84237	0	8.8725613	0.0015866	0	0	0	-85052.44	-35.548987	-683800
CaBr2(L)										
0	0	0	12.027167	0	0	0	0	-83909.323	-52.314875	-683800
CaCO3(cr)										
0	-1.33E+07	250051.72	-1907.1772	7.6166663	-0.0165587	1.88E-05	-8.72E-09	-1271058.2	9957.4976	-1206600
1	-258355.5736	0	11.972564	0.0032638	0	0	0	-149700.98	-59.611337	-1206600
CaCO3(L)										
0	0	0	19.243467	0	0	0	0	-152671.93	-105.28472	-1206600
CaCL2(cr)										
0	6000.20601	-446.61522	8.1999886	0.0237492	-1.00E-04	1.78E-07	-1.14E-10	-96060.578	-39.121596	-795800
1	-30188.18908	0	8.6447668	0.0015297	0	0	0	-98458.808	-36.842665	-795800
CaCL2(L)										
0	2661491.778	0	10.783558	0	0	0	0	-93918.186	-45.669539	-795800
CaF2(a)										
0	-987528.126	13374.267	-62.619031	0.1617894	-1.27E-04	0	0	-214604.55	361.72872	-1228000
1	-6961842.18	46920.65	-115.77082	0.1655025	-1.11E-04	3.21E-08	0	-410101.65	741.95335	-1228000
2	1.44E+09	785295.5	-13429.162	21.927831	-0.0138344	3.12E-06	0	2168972.1	78237.949	-1228000
CaF2(b)										
0	1.54E+08	0	-169.97745	0.0773312	3.59E-07	0	0	135682.87	1185.7238	-1228000
CaF2(L)										
0	0	0	11.906895	0	0	0	0	-147953.97	-59.676652	-1228000
CaH2(a)										
0	0	0	3.5997311	0.0044656	0	0	0	-22559.825	-16.861978	-177000
CaH2(b)										
0	0	0	8.2987452	0	0	0	0	-24226.336	-44.096786	-177000
CaH2(L)										
0	0	0	9.0203752	0	0	0	0	-22498.995	-47.177278	-177000
CaI2(cr)										
0	-1811328.452	31274.518	-213.6599	0.8328706	-0.0017217	1.88E-06	-8.44E-10	-210197.8	1142.8027	-536400
1	-6638.996165	0	8.652825	0.0022846	0	0	0	-67217.368	-32.543336	-536400
CaI2(L)										
0	0	0	12.387982	0	0	0	0	-64854.253	-51.372182	-536400
CaO(cr)										
0	-4775526.94	90377.114	-694.43208	2.8024772	-0.0061294	6.98E-06	-3.25E-09	-482941.14	3619.0463	-634920
1	-145937.644	0	7.1742051	-0.0019599	1.29E-06	-2.08E-10	0	-78915.251	-36.585628	-634920
CaO(L)										
0	0	0	10.10282	0	0	0	0	-79918.572	-59.0872	-634920
Ca(OH)2(cr)										
0	-205883.8935	6172.5545	-74.99751	0.5012182	-0.0014233	1.99E-06	-1.10E-09	-145202.62	355.2445	-985900
1	-124541.3139	0	10.73593	0.0039824	0	0	0	-122370.72	-53.023954	-985900
Ca(OH)2(L)										
0	0	0	18.401565	0	0	0	0	-124519.18	-98.607604	-985900
CaS(cr)										
0	4758681.13	-88407.021	667.50475	-2.5768552	0.0055273	-6.20E-06	2.85E-09	340134.47	-3494.3448	-475000
1	-14288.27435	0	5.5673756	0.0010067	0	0	0	-58881.634	-25.305724	-475000
CaS(L)										
0	0	0	8.0582019	0	0	0	0	-53485.666	-39.249955	-475000
CaSO4(II)										
0	-1.36E+07	258492.93	-1984.8006	7.9694482	-0.0173681	1.97E-05	-9.17E-09	-1334631.5	10351.394	-1434000
1	-298394.0124	0	13.596712	0.0058572	0	0	0	-177784.63	-68.024815	-1434000
CaSO4(I)										
0	0	0	19.844825	0	0	0	0	-179829.87	-104.50044	-1434000
CaSO4(L)										
0	0	0	19.844825	0	0	0	0	-176462.26	-102.55721	-1434000
Cd(cr)										
0	137527.314	-3221.5899	31.219053	-0.1226137	2.84E-04	-3.29E-07	1.52E-10	13028.069	-155.1324	0
Cd(L)										
0	0	0	3.5961229	0	0	0	0	-422.03948	-13.232982	0
Co(a)										
0	-865041.406	14618.611	-99.689311	0.3793451	-7.80E-04	8.55E-07	-3.89E-10	-67947.39	530.54307	0
1	-985661.981	6806.1641	-15.179224	0.0223031	-9.00E-06	0	0	-38448.514	101.20327	0
Co(b)										
0	0	0	2.1251138	0.0022185	0	0	0	-619.77098	-8.9445467	0
1	-1.40E+09	8165151.4	-19649.4	25.028064	-0.0177806	6.68E-06	-1.04E-09	-4.62E+07	125099.59	0
Co(b)										
0	0	0	2.1251138	0.0022185	0	0	0	-619.77098	-8.9445467	0
1	-1.40E+09	8165151.4	-19649.4	25.028064	-0.0177806	6.68E-06	-1.04E-09	-4.62E+07	125099.59	0

Co(L)										
0	0	0	4.8711229	0	0	0	0	-176.43148	-24.484351	0
Cr(cr)										
0	0	0	7.8482602	-0.116276	8.12E-04	-2.31E-06	2.35E-09	-898.01395	-27.573314	0
Cr(cr)										
0	0	0	7.8482602	-0.116276	8.12E-04	-2.31E-06	2.35E-09	-898.01395	-27.573314	0
Cr(cr)										
0	0	0	7.8482602	-0.116276	8.12E-04	-2.31E-06	2.35E-09	-898.01395	-27.573314	0
Cr(L)										
0	0	0	4.7302848	0	0	0	0	575.56338	-24.53179	0
CrN(s)										
0	0	0	9.7152904	-0.0237754	5.26E-05	-4.84E-08	1.63E-11	-16323.422	-45.73005	-117293.82
1	0	0	5.6944539	5.30E-04	2.27E-07	-8.15E-11	1.08E-14	-15836.002	-28.131704	-117293.82
Cr2N(s)										
0	0	0	2.0303388	0.0340064	-6.15E-05	5.31E-08	-1.68E-11	-16768.313	-11.600698	-125532.1
1	0	0	8.0984185	0.0018534	1.42E-06	-5.59E-10	6.93E-14	-17684.801	-39.147472	-125532.1
Cr2O3(s)										
0	0	0	29.332773	-0.1020739	2.36E-04	-2.26E-07	7.78E-11	-142404.06	-135.74281	-1135094.1
1	0	0	14.012235	0.0013824	-2.38E-07	1.70E-10	-3.77E-14	-140982.17	-71.101569	-1135094.1
Cr2O3(L)										
0	0	0	18.871105	0	0	0	0	-133694.98	-99.96147	0
Cs(cr)										
0	65198.4125	-1756.6391	19.996811	-0.0693833	1.09E-04	0	0	6382.8907	-93.382515	0
Cs(L)										
0	-42183.2769	-17.431032	5.7021247	-0.0051137	3.20E-06	-1.77E-10	4.82E-14	-1290.9498	-20.314076	0
1	-726659.499	3006.7691	0.1696419	2.91E-04	1.77E-07	7.73E-10	-8.90E-14	-19237.617	16.410037	0
CsCL(a)										
0	0	0	5.54534	0.0023806	8.36E-07	-9.96E-10	3.81E-13	-55026.535	-20.16426	-442845.67
CsCL(b)										
0	0	0	8.1610737	-0.0017624	-2.25E-07	3.93E-09	-2.35E-12	-55480.431	-33.941396	0
CsCL(L)										
0	0	0	9.3097452	0	0	0	0	-55031.161	-40.810133	0
1	0	0	9.3097452	0	0	0	0	-55031.161	-40.810133	0
CsF(s)										
0	0	0	5.6489993	0.0018711	6.62E-07	-6.31E-10	1.87E-13	-68485.102	-22.149959	-554685.85
CsF(L)										
0	0	0	8.9071617	0	0	0	0	-68066.817	-39.912774	0
1	0	0	8.9071617	0	0	0	0	-68066.817	-39.912774	0
CsOH(b)										
0	-1070491.244	27267.91	-244.79992	0.9717567	-0.0013042	0	0	-167691.52	1260.9792	-416200
1	298851.0447	0	-5.5994881	0.0475893	-3.98E-05	0	0	-49148.543	33.700832	-416200
CsOH(c)										
0	0	0	8.7437504	0	0	0	0	-51980.54	-35.917379	-416200
CsOH(L)										
0	0	0	10.223092	0	0	0	0	-51955.361	-43.898105	-416200
Cs2SO4(II)										
0	0	0	-2.9789307	0.1265088	-2.96E-04	3.32E-07	-1.31E-10	-176233.52	15.185747	-1442695.6
Cs2SO4(I)										
0	0	0	4.7349836	0.0186196	0	0	0	-171541.39	0.1373705	0
1	0	0	-0.0272327	0.031354	-1.13E-05	3.33E-09	0	-170211.63	24.839988	0
Cs2SO4(L)										
0	0	0	24.859198	0	0	0	0	-177761.98	-116.65744	0
Cu(cr)										
0	-24557.7517	164.80693	2.0809471	0.0026391	-2.71E-06	1.40E-09	-9.72E-14	-1737.851	-8.1331666	0
Cu(L)										
0	0	0	3.9449108	0	0	0	0	-211.10138	-18.360658	0
CuF(s)										
0	0	0	4.4421288	0.0079669	-7.28E-06	2.76E-09	-2.73E-13	-35336.168	-19.58517	-280337.3
1	0	0	5.3215506	0.004855	-3.54E-06	1.11E-09	-1.25E-13	-35521.715	-23.902643	-280337.3
CuF2(s)										
0	0	0	4.3873676	0.0143971	-8.62E-06	-1.98E-09	2.69E-12	-66685.585	-19.580561	-538916.63
1	0	0	2.3557676	0.0149135	-6.40E-06	0	0	-65610.622	-7.1626757	-538916.63
CuF2(L)										
0	0	0	12.077507	0	0	0	0	-63487.998	-56.73037	0
CuO(s)										
0	0	0	0.8840387	0.0241589	-4.39E-05	3.76E-08	-1.21E-11	-19788.382	-5.472388	-156065.45
1	0	0	5.0258124	0.0025424	-1.38E-06	5.35E-10	-7.97E-14	-20433.281	-24.376695	-156065.45
CuO2H2(s)										
0	0	0	10.451185	0.0013458	8.66E-06	-6.81E-09	7.44E-13	-57406.865	-47.238803	-450377.21
1	0	0	8.6730787	0.0103858	-4.70E-06	-5.03E-10	5.36E-13	-57230.382	-39.366161	-450377.21
CuSO4(s)										
0	0	0	3.3019166	0.0370123	-2.90E-05	4.53E-09	2.64E-12	-94993.621	-15.465878	-770006.8
1	0	0	11.314536	0.0140504	-1.01E-05	3.72E-09	-5.28E-13	-96998.208	-56.25469	-770006.8
Cu2O(s)										
0	0	0	3.3832466	0.0229542	-3.95E-05	3.40E-08	-1.10E-11	-22273.157	-13.530713	-170709.68
1	0	0	14.755641	-0.0158767	1.50E-05	-4.48E-09	4.06E-13	-25065.068	-70.541877	-170709.68
Cu2O(L)										
0	0	0	12.01712	0	0	0	0	-19252.387	-56.886866	0
Cu2O5S(s)										
0	0	0	2.5257178	0.072206	-9.79E-05	6.54E-08	-1.67E-11	-114786.46	-13.196112	-927626.9
1	0	0	16.011634	0.0194247	-1.84E-05	1.12E-08	-2.61E-12	-117616.2	-78.727489	-927626.9
Fe(a)										

0	13495.5994	-780.20095	9.438757	-0.0252119	5.35E-05	-5.10E-08	1.99E-11	2415.7189	-47.48269	0
1	3542934.69	-24470.873	65.608694	-0.0704377	3.18E-05	0	0	134502.45	-413.3691	0
2	2.28E+09	-5694572.2	-5624.9641	31.859455	-0.0385013	1.87E-05	-3.02E-09	4.01E+07	16217.578	0
Fe(a)										
0	13495.5994	-780.20095	9.438757	-0.0252119	5.35E-05	-5.10E-08	1.99E-11	2415.7189	-47.48269	0
1	3542934.69	-24470.873	65.608694	-0.0704377	3.18E-05	0	0	134502.45	-413.3691	0
2	2.28E+09	-5694572.2	-5624.9641	31.859455	-0.0385013	1.87E-05	-3.02E-09	4.01E+07	16217.578	0
Fe(c)										
0	9.14E+08	-3056481.7	3974.0732	-2.4220544	6.07E-04	1.24E-08	-2.20E-11	1.91E+07	-27923.087	0
Fe(d)										
0	-3.47E+08	0	709.60691	-0.547291	1.20E-04	0	0	-808986.94	-4570.0508	0
Fe(L)										
0	0	0	5.5353833	0	0	0	0	-1270.4749	-29.480968	0
FeC5O5(L)										
0	0	0	28.11845	0	0	0	0	-100524.83	-119.66541	-766109.88
1	0	0	28.11845	0	0	0	0	-100524.83	-119.66541	-766109.88
FeCL2(s)										
0	0	0	7.1122271	0.011087	-1.71E-05	1.35E-08	-4.14E-12	-43600.985	-28.994055	-341840.88
FeCL2(L)										
0	0	0	12.288863	0	0	0	0	-41109.821	-53.193057	0
1	0	0	12.288863	0	0	0	0	-41109.821	-53.193057	0
FeCL3(s)										
0	0	0	-7.3955686	0.2026084	-8.45E-04	1.59E-06	-1.08E-09	-50014.466	24.445094	-399405
FeCL3(L)										
0	0	0	16.103127	0	0	0	0	-48413.528	-67.575899	-399405
1	0	0	16.103127	0	0	0	0	-48413.528	-67.575899	-399405
FeO(s)										
0	0	0	5.3195475	0.0022097	1.07E-06	-2.79E-09	1.33E-12	-34407.165	-23.686034	-272037.03
1	0	0	5.8316489	0.0014275	-9.32E-08	-6.60E-12	-2.25E-14	-34566.902	-26.44699	-272037.03
FeO(L)										
0	0	0	8.2022482	0	0	0	0	-33848.615	-40.079129	0
Fe(OH)2(s)										
0	0	0	10.091218	0.0044523	4.07E-06	-4.01E-09	2.39E-13	-72277.688	-48.400034	-574058.56
1	0	0	7.4031808	0.0119817	-1.50E-06	-5.05E-09	2.00E-12	-71592.266	-34.673267	-574058.56
Fe(OH)3(s)										
0	0	0	4.4116836	0.0326825	-2.24E-05	2.86E-09	2.26E-12	-102718.34	-21.331014	-832627.35
1	0	0	8.0223926	0.0164201	-1.24E-07	-6.82E-09	2.33E-12	-103213.36	-37.93402	-832627.35
FeS(a)										
0	0	0	18.977627	-0.1095428	2.22E-04	0	0	-14995.242	-78.125435	-101818.26
FeS(b)										
0	0	0	8.7028505	0	0	0	0	-14689.738	-42.082102	0
FeS(c)										
0	0	0	9.3724176	9.42E-04	-1.58E-05	1.84E-08	-5.77E-12	-14581.685	-45.141516	0
1	0	0	-2.6830483	0.0367651	-5.22E-05	3.16E-08	-6.41E-12	-11498.684	16.239124	0
FeS(L)										
0	0	0	7.5232806	0	0	0	0	-10164.237	-31.97093	0
FeSO4(s)										
0	0	0	3.5057684	0.0370297	-2.90E-05	4.58E-09	2.62E-12	-114162.5	-15.223241	-928877.32
1	0	0	11.608929	0.0138047	-9.81E-06	3.61E-09	-5.10E-13	-116191.86	-56.477817	-928877.32
FeS2(s)										
0	0	0	0.4034566	0.0426747	-8.40E-05	7.63E-08	-2.54E-11	-22045.927	-5.5456393	-171549.19
1	0	0	-88.51532	0.3274893	-4.11E-04	2.29E-07	-4.78E-11	-465.12476	441.73045	-171549.19
Fe2O3(s)										
0	0	0	-7.7037843	0.1364747	-3.29E-04	3.82E-07	-1.63E-10	-100800.76	25.292085	-825315.2
1	0	0	40.49753	-0.0461316	3.18E-05	-8.92E-09	8.47E-13	-113176.27	-216.35088	-825315.2
Fe2S3O12(s)										
0	0	0	11.116955	0.0837068	-4.14E-05	-2.53E-08	2.10E-11	-317297.82	-49.28875	-2583054.5
1	0	0	39.114438	0.0117963	-3.39E-08	-2.30E-09	6.41E-13	-324782.62	-194.00429	-2583054.5
Fe3O4(s)										
0	0	0	36.198148	-0.1743798	5.25E-04	-5.42E-07	1.80E-10	-141387.3	-155.56683	-1119932.4
1	0	0	24.13372	4.16E-05	-2.63E-08	6.60E-12	-5.69E-16	-141210.52	-120.06412	-1119932.4
Ga(cr)										
0	1665.524651	-166.7536	3.8608764	-0.0013254	2.41E-06	0	0	-157.77919	-17.30178	0
Ga(L)										
0	28468.30421	0	3.1353622	-3.62E-05	2.90E-08	0	0	-171.64967	-10.537173	0
GaBr3(cr)										
0	0	0	3.563409	0.0279843	0	0	0	-48851.378	-6.9974953	-387000
GaBr3(L)										
0	0	0	15.442882	0	0	0	0	-49906.951	-63.308017	-387000
GaCL3(cr)										
0	0	0	2.7254763	0.0295844	0	0	0	-65510.701	-8.2328575	-527000
GaCL3(L)										
0	0	0	13.109612	0	0	0	0	-65994.494	-54.894181	-527000
GaF3(cr)										
0	0	0	9.361586	0.0045032	0	0	0	-144310.52	-43.135094	-1175000
GaI3(cr)										
0	0	0	6.4617157	0.0186668	0	0	0	-28975.461	-17.726054	-218000
GaI3(L)										
0	0	0	16.561409	0	0	0	0	-30126.863	-67.931701	-218000
Ga2O3(cr)										
0	-1.52E+07	278792.24	-2090.0938	8.2368547	-0.0177141	1.99E-05	-9.17E-09	-1391968.8	10942.213	-1091000
1	-285753.4599	0	13.758838	0.0017995	0	0	0	-136357.04	-70.320817	-1091000

Ga2O3(L)										
0	0	0	19.243467	0	0	0	0	-131707.84	-102.66577	-1091000
Ge(cr)										
0	-239650.371	3150.5687	-13.339396	0.0364799	-2.94E-05	0	0	-16138.813	79.392016	0
1	-18882.4135	0	2.898173	3.59E-04	0	0	0	-943.38639	-12.986697	0
Ge(L)										
0	0	0	3.3194981	0	0	0	0	3278.9966	-11.85993	0
GeO2(II)										
0	-13620.6101	0	1.390091	0.0160881	0	0	0	-70956.827	-8.0174837	-580200
1	-276312.1338	0	9.4046432	-0.0012122	1.11E-06	0	0	-73468.301	-50.049971	-580200
GeO2(I)										
0	-153526.7863	0	7.48186	0.0017115	0	0	0	-69946.53	-37.11332	-580200
GeO2(L)										
0	0	0	9.4413261	0	0	0	0	-68838.379	-47.385512	-580200
GeS(cr)										
0	-17538.90915	0	4.9670492	0.0032771	0	0	0	-10747.639	-21.380308	-75348
1	0	0	5.0153286	0.0024535	0	0	0	-10666.602	-21.311183	-75348
GeS(L)										
0	0	0	8.0582019	0	0	0	0	-9874.413	-37.077155	-75348
GeS2(cr)										
0	-22395.38329	0	5.7542	0.0080482	0	0	0	-16761.455	-24.053234	-121500
1	-33676.0675	0	7.8898215	0.001311	0	0	0	-17136.576	-34.275874	-121500
GeS2(L)										
0	0	0	12.027167	0	0	0	0	-18938.767	-60.064501	-121500
HBO2(cr)										
0	0	0	4.478917	0.0070455	0	0	0	-98419.124	-21.726371	-804600
HBO2(L)										
0	0	0	12.628525	0	0	0	0	-99934.711	-65.553266	-804600
H2O(s)										
0	-389736.288	2415.022	60.941907	-0.8470311	0.0044777	-1.07E-05	9.77E-09	-53915.062	-207.59648	-299108
H2O(L)										
0	8.72E+07	-1390875.1	9157.2953	-31.759635	0.0613885	-6.27E-05	2.65E-08	6433165.2	-49098.532	-285830
H2SO4(L)										
0	0	0	9.9421525	0.0217864	3.50E-06	-3.35E-09	1.17E-12	-101859.79	-44.398695	-814010.34
H3BO3(cr)										
0	2370260.101	-31164.266	148.81407	-0.2710868	2.27E-04	0	0	19508.118	-857.5442	-1094800
H3BO3(L)										
0	0	0	21.648901	0	0	0	0	-136742.66	-110.09103	-1094800
H3PO4(cr)										
0	2733.365471	0	1.1093479	0.0412902	-7.81E-06	0	0	-156575.32	-4.9734731	-1284488
H3PO4(L)										
0	41090.8111	-441.03435	8.5477917	0.0319826	5.17E-06	-3.26E-09	8.32E-13	-154317.54	-41.553987	-1284488
Hg(cr)										
0	-3184.58668	0	3.4644249	-0.0040549	1.77E-05	0	0	-1282.4543	-11.320102	0
Hg(L)										
0	105832.237	-1993.8212	18.805738	-0.0599467	1.23E-04	-1.29E-07	5.53E-11	7916.7553	-90.648533	0
1	791380.154	-3956.305	11.064608	-0.0081539	4.97E-06	-1.51E-09	1.87E-13	22137.599	-60.72429	0
HgBr2(s)										
0	0	0	8.2829714	0.0016302	3.42E-06	7.10E-10	-4.34E-12	-22952.438	-27.345276	-169456.46
HgBr2(L)										
0	0	0	12.278799	0	0	0	0	-22500.898	-46.851212	0
1	0	0	12.278799	0	0	0	0	-22500.898	-46.851212	0
HgO(s)										
0	0	0	3.4170866	0.0071161	-1.49E-06	-4.49E-09	2.59E-12	-12233.27	-13.037185	-90786.065
I2(cr)										
0	-3915902.52	91754.647	-892.97865	4.6853413	-0.0136092	2.08E-05	-1.30E-08	-392659.65	4437.3817	0
I2(L)										
0	0	0	9.5682127	0	0	0	0	-1204.4538	-36.373261	0
In(cr)										
0	8511.61687	-345.047	6.8387852	-0.0181853	4.12E-05	-2.96E-08	0	458.059	-29.289142	0
In(L)										
0	50923.02493	0	3.302179	-1.31E-04	6.04E-08	0	0	-451.15176	-10.750158	0
InBr(cr)										
0	0	0	4.6335863	0.0046285	0	0	0	-22634.769	-14.55042	-175000
InBr(L)										
0	0	0	8.4190169	0	0	0	0	-22222.385	-32.67501	-175000
InBr3(cr)										
0	0	0	11.541149	0.0024368	0	0	0	-51537.699	-45.43581	-399000
InBr3(L)										
0	0	0	16.236675	0	0	0	0	-51079.494	-69.948312	-399000
InCL(crII)										
0	0	0	5.1639844	0.0034386	0	0	0	-24123.141	-18.420342	-186500
InCL(crI)										
0	0	0	6.7352135	0	0	0	0	-24411.17	-26.290062	-186500
InCL(L)										
0	0	0	8.0582019	0	0	0	0	-22489.71	-29.175941	-186500
InCl3(cr)										
0	0	0	10.934379	0.0036652	0	0	0	-67166.974	-46.313869	-530000
InCl3(L)										
0	0	0	14.071785	0	0	0	0	-65262.462	-60.567497	-530000
InF3(cr)										
0	0	0	9.7517472	0.0044043	0	0	0	-146226.53	-43.644796	-1190000

InF3(L)										
0	0	0	16.116404	0	0	0	0	-143127.88	-78.26198	-1190000
InI(cr)										
0	-92539.7672	1215.1338	-0.0103888	0.0136879	-9.12E-06	1.60E-09	1.52E-12	-20090.172	14.365986	-102500
InI(L)										
0	0	0	8.4430712	0	0	0	0	-13319.499	-31.684757	-102500
InI2(crII)										
0	26574.10907	0	6.9462102	0.0068899	0	0	0	-23455.929	-20.566208	-176000
InI2(crI)										
0	0	0	10.805207	0	0	0	0	-24383.46	-40.709506	-176000
InI2(L)										
0	0	0	13.795161	0	0	0	0	-24444.248	-56.405259	-176000
InI3(cr)										
0	-1888.265213	0	10.964687	0.0048045	0	0	0	-30429.853	-37.082836	-224000
InI3(L)										
0	0	0	16.525327	0	0	0	0	-30318.928	-64.472327	-224000
In2O3(cr)										
0	-9503707.35	177090.75	-1344.5037	5.3913037	-0.0117177	1.33E-05	-6.16E-09	-910473.37	7021.3392	-923000
1	-271994.3809	0	14.614331	0.0012102	0	0	0	-116334.07	-72.913898	-923000
In2O3(L)										
0	0	0	19.243467	0	0	0	0	-110808.95	-100.06026	-923000
K(cr)										
0	-102203.174	0	13.33752	-0.0558099	9.01E-05	0	0	-2635.0624	-56.153765	0
K(L)										
0	-3935.79278	-45.472287	4.8452427	-0.0030835	2.02E-06	-3.71E-11	5.03E-15	-807.5637	-18.366409	0
KCN(s)										
0	0	0	8.1799728	-0.0014011	3.42E-06	-3.50E-09	1.31E-12	-16048.201	-30.944525	-113473.6
KCN(L)										
0	0	0	9.0581305	0	0	0	0	-15226.717	-35.454083	0
1	0	0	9.0581305	0	0	0	0	-15226.717	-35.454083	0
KCL(s)										
0	0	0	5.3934311	0.0026535	9.61E-07	-5.03E-09	4.07E-12	-54248.389	-21.596814	-436694.01
1	0	0	3.9157169	-0.0020927	4.73E-06	7.02E-09	-5.51E-12	-52747.066	-10.1448	-436694.01
KCL(L)										
0	0	0	8.8518064	0	0	0	0	-53369.478	-40.010059	0
KF(s)										
0	0	0	4.9843972	0.0035943	-1.77E-06	-4.81E-10	1.03E-12	-70018.149	-21.384504	-568616
1	0	0	9.4627782	-0.0064058	6.39E-08	7.59E-09	-3.36E-12	-71249.107	-44.831804	-568616
KF(L)										
0	0	0	8.6555469	0	0	0	0	-69268.025	-41.179932	0
KHF2(a)										
0	0	0	-9.1298498	0.0866189	4.39E-05	-6.69E-07	8.05E-10	-112582.59	41.0828	-931297.73
KHF2(b)										
0	0	0	12.057378	0	0	0	0	-114571.26	-54.17014	0
KHF2(L)										
0	0	0	12.580737	0	0	0	0	-114043.09	-55.879915	0
1	0	0	12.580737	0	0	0	0	-114043.09	-55.879915	0
KOH(a)										
0	-438006.462	11254.729	-102.36233	0.437563	-5.92E-04	0	0	-100215.58	524.13083	-423400
KOH(b)										
0	-2814.35707	0	6.4783132	0.0061838	0	0	0	-53138.822	-28.998263	-423400
KOH(c)										
0	0	0	9.6217336	0	0	0	0	-53258.578	-44.133467	-423400
KOH(L)										
0	0	0	10.463635	0	0	0	0	-52880.083	-48.223857	-423400
KO2(s)										
0	0	0	3.8775487	0.030157	-5.12E-05	4.16E-08	-1.31E-11	-36340.727	-14.419032	-284525.34
1	0	0	-10.494545	0.068859	-8.14E-05	4.29E-08	-8.50E-12	-32489.989	59.685913	-284525.34
K2CO3(s)										
0	0	0	8.4398632	0.0188363	-4.68E-07	-1.05E-08	6.43E-12	-141667.44	-34.894424	-1150194.2
1	0	0	22.824341	-0.013581	8.74E-06	1.15E-08	-6.76E-12	-145778.44	-110.48665	-1150194.2
K2CO3(L)										
0	0	0	25.161469	0	0	0	0	-147401.38	-131.1073	0
K2O(s)										
0	0	0	0.4430399	0.0620638	-1.36E-04	1.36E-07	-4.90E-11	-45612.586	-4.7590347	-363171
1	0	0	7.1870264	0.0091149	-4.18E-06	1.80E-09	-2.84E-13	-46000.943	-31.74498	-363171
K2O2(s)										
0	0	0	8.8267421	0.0132621	-1.11E-05	1.10E-08	-4.24E-12	-62773.525	-40.251432	-495804
1	0	0	10.48163	0.0069086	4.87E-07	-2.55E-10	4.08E-14	-63181.432	-48.47729	-495804
K2S(1)										
0	0	0	31.364431	-0.1881066	5.60E-04	-6.97E-07	3.12E-10	-49997.406	-128.10455	-376553.66
1	0	0	-74.849337	0.0936198	0	0	0	-9721.7939	449.67393	-376553.66
K2S(2)										
0	0	0	156.42816	-0.1266444	0	0	0	-131144.19	-927.94275	0
K2S(3)										
0	0	0	17.119867	0	0	0	0	-54524.953	-91.666511	0
K2S(L)										
0	0	0	12.142927	0	0	0	0	-46520.349	-54.716043	0
K2SO4(a)										
0	0	0	1.7026526	0.0847097	-1.76E-04	1.93E-07	-7.65E-11	-175980.87	-7.5631951	-1437753.5
K2SO4(b)										
0	0	0	13.807177	0.0096731	4.57E-08	0	0	-175853.26	-58.441296	0

1	0	0	-290.19866	1.0569631	-0.0013475	7.68E-07	-1.63E-10	-105542.14	1453.0094	0
K2SO4(L)										
0	0	0	24.230499	0	0	0	0	-176955.19	-117.40222	0
Li(cr)										
0	-9860.65231	0	2.3043239	0.0026717	0	0	0	-838.85361	-10.478817	0
1	72388.2507	0	0.1570314	0.0067704	0	0	0	-104.94973	0.9961764	0
Li(L)										
0	24655.6923	0	3.7557234	-6.33E-04	3.16E-07	0	0	-729.91167	-17.012747	0
LiALO2(s)										
0	0	0	-5.2841156	0.0784526	-1.45E-04	1.25E-07	-4.01E-11	-143818.31	18.576733	-1188677.1
1	0	0	8.5440894	0.0064887	-4.09E-06	1.55E-09	-2.25E-13	-145981.5	-44.590618	-1188677.1
LiALO2(L)										
0	0	0	15.096679	0	0	0	0	-141658.39	-80.993767	0
LiCL(s)										
0	0	0	4.1095245	0.0081981	-1.15E-05	1.06E-08	-3.65E-12	-50608.266	-18.298894	-408254.13
LiCL(L)										
0	0	0	10.383028	-0.004718	-1.61E-06	8.08E-09	-4.45E-12	-50539.12	-49.92196	0
1	0	0	8.2149477	5.64E-04	-1.74E-06	7.66E-10	-1.24E-13	-50007.322	-38.808961	0
LiF(s)										
0	0	0	1.7694325	0.0175052	-2.80E-05	2.29E-08	-6.96E-12	-75299.278	-9.9478057	-616931.95
1	0	0	5.5405738	-1.34E-04	1.78E-06	8.90E-10	-9.13E-13	-75900.365	-27.447276	-616931.95
LiF(L)										
0	0	0	7.7195401	0	0	0	0	-74304.347	-38.815487	0
LiH(s)										
0	0	0	0.3861181	0.012128	-8.69E-06	5.63E-09	-1.27E-12	-11486.991	-3.0654575	-90620.411
LiH(L)										
0	0	0	7.4981191	0	0	0	0	-11581.826	-40.047278	0
1	0	0	7.4981191	0	0	0	0	-11581.826	-40.047278	0
LiOH(cr)										
0	-1219595.668	20883.151	-146.34755	0.5611591	-0.0010844	1.07E-06	-4.22E-10	-155353.47	774.41292	-487500
LiOH(L)										
0	0	0	10.499717	0	0	0	0	-60502.807	-54.07388	-487500
Li2O(s)										
0	0	0	-0.3172724	0.0361494	-5.55E-05	4.18E-08	-1.18E-11	-73106.196	-2.288833	-598702.84
1	0	0	4.2774776	0.0078522	-5.22E-07	-1.79E-09	5.40E-13	-73396.278	-21.765497	-598702.84
Li2O(L)										
0	0	0	12.076931	0	0	0	0	-71337.921	-65.174974	0
Li2SO4(a)										
0	0	0	-4.138736	0.1069406	-2.09E-04	2.13E-07	-8.02E-11	-174806.78	12.983577	-1436367
Li2SO4(b)										
0	0	0	25.795481	-2.85E-04	1.53E-07	0	0	-180308.45	-136.31217	-1436367
1	0	0	26.102651	-8.29E-04	3.91E-07	0	0	-180422.45	-138.0081	-1436367
Li2SO4(L)										
0	0	0	24.657913	0	0	0	0	-178097.8	-127.62616	-1436367
Li3N(s)										
0	0	0	2.9225558	0.0285987	-3.53E-05	3.19E-08	-1.11E-11	-21678.029	-16.331057	-164544.31
1	0	0	5.4422503	0.0134777	-1.94E-06	-2.50E-11	0	-22015.776	-27.457275	-164544.31
Mg(cr)										
0	-5412.225134	0	1.4581737	0.013302	-4.10E-05	4.75E-08	0	-775.9472	-6.9897023	0
1	-28600.60304	0	3.3988774	-7.24E-04	1.41E-06	0	0	-1089.5199	-15.459737	0
Mg(L)										
0	0	0	4.1253183	0	0	0	0	-658.99195	-19.378286	0
MgAL2O4(s)										
0	0	0	-6.3912625	0.1171886	-2.13E-04	1.83E-07	-5.88E-11	-278271.41	20.132701	-2299119.5
1	0	0	14.697679	0.0093305	-3.55E-06	1.16E-09	-1.43E-13	-281664.11	-76.668685	-2299119.5
MgAL2O4(L)										
0	0	0	26.419188	0	0	0	0	-268835.36	-141.98581	0
MgBr2(cr)										
0	-66570.36915	0	9.124771	0.0014433	0	0	0	-66270.875	-38.722227	-526000
MgBr2(L)										
0	0	0	12.027167	0	0	0	0	-63633.781	-52.466377	-526000
MgCO3(cr)										
0	-5649471.92	105980.93	-809.59538	3.2679927	-0.0071116	8.09E-06	-3.76E-09	-609852.85	4221.968	-1096000
1	-174333.7852	0	8.8201229	0.0076962	0	0	0	-135374.26	-45.700398	-1096000
MgCO3(L)										
0	0	0	18.04075	0	0	0	0	-133647.49	-96.153843	-1096000
MgCL2(cr)										
0	315127.1437	-4986.5617	34.074904	-0.0601333	7.26E-05	-2.98E-08	-5.06E-12	-56089.094	-183.34158	-644300
1	-77454.95525	0	9.0991532	0.0011997	0	0	0	-80517.07	-41.857958	-644300
MgCL2(L)										
0	712008.2843	0	10.601226	0	0	0	0	-75431.685	-45.372959	-644300
MgF2(cr)										
0	-8758857.47	163069.03	-1234.7845	4.9131144	-0.010644	1.20E-05	-5.57E-09	-871037.95	6452.7217	-1124200
1	-186360.9521	0	9.3583386	4.87E-04	0	0	0	-138646.3	-47.63421	-1124200
MgF2(L)										
0	0	0	11.401754	0	0	0	0	-134053.16	-57.258281	-1124200
MgH2(b)										
0	4034912.2	-61154.008	353.70843	-0.9554057	0.0012605	-6.39E-07	0	279992.02	-1959.4912	-75700
MgH2(L)										
0	0	0	9.0203752	0	0	0	0	-11350.517	-47.771946	-75700
MgI2(cr)										
0	0	0	8.2915289	0.0022327	0	0	0	-47071.874	-31.791071	-370000

MgI2(L)										
0	0	0	12.027167	0	0	0	0	-46412.949	-51.752825	-370000
MgO(cr)										
0	-898078.457	17712.454	-144.93257	0.6397591	-0.0014583	1.72E-06	-8.18E-10	-151629.09	743.90097	-601600
1	-116952.1716	0	5.5103668	0.0010859	-4.87E-07	1.25E-10	0	-74434.827	-29.115649	-601600
MgO(L)										
0	0	0	10.10282	0	0	0	0	-76093.708	-60.76894	-601600
Mg(OH)2(cr)										
0	-640145.184	8358.14	-39.711454	0.1231927	-9.65E-05	0	0	-153724.69	225.84954	-924350
1	-5543828.43	37008.686	-90.886233	0.1431689	-9.51E-05	2.53E-08	0	-318945.09	580.16383	-924350
Mg(OH)2(L)										
0	-303758.1289	0	12.034624	0.0022027	0	0	0	-115877.55	-63.338526	-924350
MgS(cr)										
0	1862529.34	-35369.41	272.18397	-1.0429077	0.0022467	-2.53E-06	1.16E-09	115712.2	-1421.7764	-348000
1	-27746.67419	0	5.4776529	0.0010532	0	0	0	-43627.578	-25.626215	-348000
MgS(L)										
0	0	0	8.0582019	0	0	0	0	-39199.428	-40.150435	-348000
MgSO4(II)										
0	7038799.19	-128386.69	946.49558	-3.5621171	0.0075358	-8.35E-06	3.80E-09	424356.62	-4979.3775	-1288800
1	-140369.0656	0	10.244741	0.0105328	-2.38E-06	0	0	-158978.51	-51.17736	-1288800
MgSO4(I)										
0	0	0	18.642109	0	0	0	0	-162291.71	-99.401975	-1288800
MgSO4(L)										
0	0	0	18.642109	0	0	0	0	-160535.74	-98.156609	-1288800
MgSiO3(I)										
0	0	0	1.3377779	0.0444532	-6.60E-05	4.74E-08	-1.23E-11	-188172.26	-10.178936	-1548931.6
MgSiO3(II)										
0	0	0	14.473886	0	0	0	0	-191621.72	-76.659464	0
1	0	0	14.473886	0	0	0	0	-191621.72	-76.659464	0
MgSiO3(III)										
0	0	0	14.725501	0	0	0	0	-191741.99	-78.299298	0
MgSiO3(L)										
0	0	0	17.613031	0	0	0	0	-188025.79	-95.125731	0
MgTiO3(s)										
0	0	0	-0.1577774	0.0620184	-1.05E-04	8.49E-08	-2.64E-11	-191077.38	-4.6616535	-1572593.5
1	0	0	10.288224	0.0103437	-7.40E-06	2.79E-09	-3.95E-13	-192811.68	-52.958088	-1572593.5
MgTiO3(L)										
0	0	0	19.625949	0	0	0	0	-190918.12	-106.56204	0
MgTi2O5(s)										
0	0	0	1.2716311	0.0926638	-1.64E-04	1.39E-07	-4.45E-11	-305116.13	-12.422102	-2509409.5
1	0	0	16.776608	0.0122378	-6.30E-06	2.40E-09	-3.54E-13	-307546.55	-83.29339	-2509409.5
MgTi2O5(L)										
0	0	0	31.401519	0	0	0	0	-304100.01	-168.58649	0
Mg2SiO4(s)										
0	0	0	1.3428982	0.0668666	-9.64E-05	6.64E-08	-1.72E-11	-264469.01	-12.399162	-2176951.2
1	0	0	15.752679	0.0068005	-1.62E-06	7.74E-12	6.33E-14	-267299.55	-81.457992	-2176951.2
Mg2SiO4(L)										
0	0	0	24.658244	0	0	0	0	-266925.49	-134.6151	0
Mg2TiO4(s)										
0	0	0	-0.0504412	0.0880864	-1.57E-04	1.34E-07	-4.31E-11	-263078.65	-6.2537507	-2164430.7
1	0	0	14.772577	0.0108241	-4.99E-06	1.74E-09	-2.54E-13	-265390.78	-73.93371	-2164430.7
Mg2TiO4(L)										
0	0	0	27.476329	0	0	0	0	-261535.59	-147.45837	0
Mg3N2(cr)										
0	-331312.3684	0	14.489128	0.0010357	0	0	0	-60958.514	-74.502435	-461300
Mn(a)										
0	-19847.2475	180.88143	1.0382897	0.0088133	-1.30E-05	1.12E-08	-3.67E-12	-1704.1431	-3.7131605	0
Mn(b)										
0	-2.07E+08	874475.49	-1470.4334	1.2395222	-5.19E-04	8.67E-08	0	-5242434.7	9928.234	0
Mn(c)										
0	-5539098.66	0	12.491411	-0.0031726	0	0	0	-13193.66	-77.007474	0
Mn(d)										
0	-4256308.77	0	10.012464	-0.0017265	0	0	0	-10000.477	-60.588391	0
Mn(L)										
0	0	0	5.5353833	0	0	0	0	-939.37688	-28.535703	0
Mo(cr)										
0	-49616.8936	428.09412	0.7671984	0.0057315	-6.38E-06	3.71E-09	-7.92E-13	-3039.5847	-1.2304675	0
1	-3614786.56	14734.788	-21.347027	0.0211682	-9.78E-06	2.49E-09	-2.42E-13	-89709.247	150.58364	0
2	3.27E+09	-1774787.1	-4389.9552	5.6493962	-0.0026809	5.84E-07	-4.89E-11	1.77E+07	25600.419	0
Mo(L)										
0	0	0	4.52895	0	0	0	0	2022.3185	-22.80791	0
NH4CL(a)										
0	0	0	4.6749383	0.0192734	0	0	0	-40082.751	-20.959133	-314556.85
NH4CL(b)										
0	0	0	4.166685	0.013436	0	0	0	-38762.693	-14.134402	-314556.85
NH4F(cr)										
0	-2246351.51	54108.77	-550.705	3.0758881	-0.0095981	1.62E-05	-1.15E-08	-286367.75	2704.3292	-467560
1	0	0	1.5635317	0.0210848	0	0	0	-57637.54	-6.538862	-467560
NH4F(L)										
0	0	0	13.590699	0	0	0	0	-59515.154	-67.804771	-467560
Na(cr)										
0	-35844.5796	0	6.4794147	-0.018987	3.35E-05	0	0	-1504.3197	-26.77783	0

Na(L)										
0	26948.3872	-231.90139	5.162439	-0.0030586	1.70E-06	-1.52E-10	1.96E-14	284.21876	-22.257661	0
NaALO2(a)										
0	0	0	-0.8050478	0.058435	-1.19E-04	1.20E-07	-4.62E-11	-137816.65	-0.0533353	-1133223.4
NaALO2(b)										
0	0	0	10.542343	8.85E-04	1.39E-06	-5.14E-10	0	-139580.6	-52.371362	0
1	0	0	11.966215	-0.0022817	3.77E-06	-1.29E-09	1.41E-13	-140048.18	-60.006455	0
NaBr(s)										
0	0	0	4.8766461	0.0068319	-1.06E-05	9.16E-09	-2.88E-12	-45148.644	-18.982545	-361417.5
1	0	0	6.6246448	1.24E-04	4.10E-07	2.07E-10	-1.81E-14	-45560.372	-27.6058	-361417.5
NaBr(L)										
0	0	0	7.4981191	0	0	0	0	-43049.77	-30.170451	0
NaCN(s)										
0	0	0	7.9967732	0.0019155	-5.34E-06	6.81E-09	-3.14E-12	-13340.294	-31.703933	-90679.248
NaCN(L)										
0	0	0	9.56136	0	0	0	0	-13386.407	-40.287309	0
1	0	0	9.56136	0	0	0	0	-13386.407	-40.287309	0
NaCL(s)										
0	0	0	5.0240778	0.0051949	-7.28E-06	6.07E-09	-1.20E-12	-51123.335	-21.227201	-411131.19
1	0	0	2.2134927	0.001586	5.05E-06	2.60E-09	-3.65E-12	-49263.203	-2.602566	-411131.19
NaCL(L)										
0	0	0	12.358488	-0.0063071	3.20E-06	-6.77E-10	5.10E-14	-51423.265	-60.58553	0
NaF(s)										
0	0	0	3.6977552	0.0105206	-1.72E-05	1.41E-08	-3.95E-12	-70647.183	-17.393633	-575391.67
1	0	0	7.8342026	-9.48E-04	-5.48E-06	8.68E-09	-2.93E-12	-71810.405	-38.81571	-575391.67
NaF(L)										
0	0	0	10.963261	-0.0032068	1.16E-06	-1.63E-10	5.25E-15	-70673.943	-56.375695	0
NaI(s)										
0	0	0	5.4995984	0.0035668	-4.00E-06	3.18E-09	-9.53E-13	-36390.356	-20.399251	-287861.51
NaI(L)										
0	0	0	7.8000568	0	0	0	0	-34759.568	-30.818881	0
1	0	0	7.8000568	0	0	0	0	-34759.568	-30.818881	0
NaOH(a)										
0	20083.29119	-771.46772	8.6941711	0.0038509	-3.61E-06	0	0	-49480.235	-45.248996	-425800
1	1048215.71	0	-95.928924	0.6189565	-0.0013672	1.07E-06	0	-36635.41	427.00511	-425800
NaOH(b)										
0	0	0	9.6217336	0	0	0	0	-54425.59	-47.992926	-425800
NaOH(c)										
0	0	0	10.343364	0	0	0	0	-54070.548	-51.222887	-425800
NaOH(L)										
0	0	0	10.777905	-7.11E-04	0	0	0	-53438.275	-52.288061	-425800
1	0	0	10.066739	0	0	0	0	-53082.692	-48.086664	-425800
NaO2(s)										
0	0	0	7.2798882	0.0044161	1.24E-06	-1.29E-09	4.83E-13	-33726.561	-28.899807	-260669.37
1	0	0	6.6753177	0.0064235	-1.54E-06	6.84E-10	-1.11E-13	-33572.546	-25.848608	-260669.37
Na2CO3(I)										
0	0	0	6.7835659	0.0388297	-9.83E-05	1.65E-07	-8.33E-11	-139170.1	-30.463293	-1130792.2
Na2CO3(II)										
0	0	0	11.848341	-0.0035139	2.06E-05	-7.40E-09	0	-138141.87	-48.064368	0
1	0	0	8.2817755	0.0112754	2.00E-06	0	0	-137612.66	-31.37258	0
Na2CO3(L)										
0	0	0	22.796295	0	0	0	0	-142292.18	-116.22121	0
Na2O(c)										
0	0	0	5.2654583	0.0111169	-6.39E-07	-9.70E-09	5.37E-12	-52314.345	-24.187024	-417992.14
1	0	0	24.168956	-0.0252797	-4.74E-06	3.18E-08	-1.46E-11	-58048.236	-125.18065	-417992.14
Na2O(a)										
0	0	0	-149.0659	0.2279904	3.84E-05	-1.71E-07	6.14E-11	11614.795	846.89268	0
Na2O(L)										
0	0	0	12.580737	0	0	0	0	-48594.857	-60.661549	0
Na2O2(a)										
0	0	0	4.5815278	0.0324559	-5.12E-05	4.27E-08	-1.40E-11	-64161.053	-22.455453	-513227.64
Na2O2(b)										
0	0	0	13.66268	0	0	0	0	-65632.571	-66.841551	0
1	0	0	13.66268	0	0	0	0	-65632.571	-66.841551	0
Na2S(1)										
0	0	0	9.7075599	-3.11E-04	5.51E-06	-6.04E-09	2.30E-12	-46950.379	-43.837613	-366105.02
1	0	0	446.7556	-1.0585111	8.12E-04	-1.89E-07	0	-177483.94	-2346.2659	-366105.02
Na2S(2)										
0	0	0	-567935.49	1680.4121	-1.8622679	9.16E-04	-1.69E-07	1.53E+08	2910868.7	0
Na2S(L)										
0	0	0	11.071048	0	0	0	0	-42790.93	-48.615889	0
Na2SO3(s)										
0	0	0	12.901936	0.0052335	0	0	0	-136474.62	-57.518193	-1100802
Na2SO3(L)										
0	0	0	21.889925	0	0	0	0	-140338.22	-112.30003	-1100802
Na2SO4(V)										
0	0	0	5.8339319	0.0308202	5.98E-05	-2.60E-07	2.48E-10	-170156.08	-25.288643	-1387816
Na2SO4(IV)										
0	0	0	9.7196778	0.021882	-6.20E-06	0	0	-170712.82	-43.606337	-1387816
Na2SO4(I)										
0	0	0	15.485439	0.0192614	-3.32E-05	3.56E-08	-1.31E-11	-171322.92	-73.512702	-1387816
1	0	0	16.115739	0.0082093	-2.33E-07	0	0	-171129.1	-74.699075	-1387816

Na2SO4(L)										
0	0	0	23.697773	0	0	0	0	-171658.91	-116.35848	-1387816
Na3ALF6(a)										
0	0	0	2.2592958	0.1556967	-3.62E-04	4.05E-07	-1.65E-10	-404059.93	-17.798545	-3316981.9
Na3ALF6(b)										
0	0	0	16.593657	0.0169117	1.03E-06	0	0	-401086.89	-64.910792	0
1	0	0	9.5543957	0.0352015	-1.46E-05	4.40E-09	0	-399075.52	-28.216177	0
Na3ALF6(L)										
0	0	0	47.567623	0	0	0	0	-412965.38	-253.7588	0
Na5AL3F14(s)										
0	0	0	13.728171	0.232983	-4.17E-04	3.54E-07	-1.13E-10	-923255.82	-73.913754	-7581530.3
1	0	0	60.805376	0.010149	0	0	0	-931943.65	-294.91948	-7581530.3
Na5AL3F14(L)										
0	0	0	117.1301	0	0	0	0	-956128.84	-647.05309	0
Nb(cr)										
0	-42548.1221	387.52978	1.1844493	0.0045074	-5.23E-06	3.51E-09	-9.51E-13	-2864.4497	-2.4429728	0
1	2.53E+07	-108492.69	192.77608	-0.1726113	8.66E-05	-2.26E-08	2.44E-12	646758.66	-1283.088	0
2	-1.35E+09	3880052.9	-4560.6795	2.8170756	-9.63E-04	1.73E-07	-1.27E-11	-2.47E+07	32328.36	0
Nb(L)										
0	0	0	4.0257333	0	0	0	0	1427.0532	-18.579649	0
NbO(s)										
0	0	0	2.982126	0.0102175	-1.52E-05	1.13E-08	-3.14E-12	-51703.369	-13.918597	-419661.16
1	0	0	5.1236553	8.94E-04	3.09E-07	-1.64E-10	2.86E-14	-52110.91	-24.09952	-419661.16
NbO(L)										
0	0	0	7.5484421	0	0	0	0	-44587.138	-35.81734	0
NbOCL3(cr)										
0	-182230.4138	482.85934	13.418611	0.0075465	-1.20E-05	1.00E-08	-3.43E-12	-113389.74	-60.579734	-879500
NbO2(I)										
0	0	0	-1.5484179	0.0545536	-1.21E-04	1.24E-07	-4.56E-11	-96731.163	3.4726822	-794960
1	0	0	5.2890272	0.0052039	0	0	0	-97297.246	-24.89086	-794960
NbO2(II)										
0	0	0	11.17141	0	0	0	0	-100206	-59.981944	-794960
NbO2(III)										
0	0	0	9.9888508	0	0	0	0	-98786.927	-51.597509	-794960
NbO2(L)										
0	0	0	11.322375	0	0	0	0	-90616.576	-56.755346	-794960
Nb2O5(s)										
0	0	0	8.5053488	0.0344012	-3.77E-05	1.99E-08	-3.96E-12	-232232.29	-40.68492	-1899558.5
1	0	0	17.054892	0.0049141	4.73E-07	-1.84E-09	5.06E-13	-234230.27	-83.224799	-1899558.5
Nb2O5(L)										
0	0	0	29.136987	0	0	0	0	-237360.25	-159.33396	0
Ni(cr)										
0	-768691.897	14335.636	-104.24769	0.3925317	-6.99E-04	4.91E-07	0	-65419.974	550.99283	0
1	-3.33E+08	3410969.8	-13890.671	28.151382	-0.0283754	1.14E-05	0	-1.74E+07	81482.639	0
Ni(cr)										
0	-768691.897	14335.636	-104.24769	0.3925317	-6.99E-04	4.91E-07	0	-65419.974	550.99283	0
1	-3.33E+08	3410969.8	-13890.671	28.151382	-0.0283754	1.14E-05	0	-1.74E+07	81482.639	0
Ni(L)										
0	0	0	4.6798909	0	0	0	0	-321.61781	-23.354766	0
NiS(b)										
0	0	0	2.5150513	0.0198109	-4.48E-05	5.36E-08	-2.47E-11	-11897.275	-12.298805	-87868.633
NiS(a)										
0	0	0	1.5977855	0.0162792	-2.40E-05	1.97E-08	-6.00E-12	-10605.192	-4.9988414	0
1	0	0	-2.1688277	0.0204673	-1.52E-05	4.52E-09	0	-9253.9731	16.018976	0
NiS(L)										
0	0	0	9.2342608	0	0	0	0	-11053.652	-45.769736	0
NiS2(s)										
0	0	0	7.7449349	0.0025352	-9.98E-08	1.08E-10	-4.19E-14	-18222.539	-36.224388	-131380.86
1	0	0	5.274264	0.0090871	-5.82E-06	1.71E-09	0	-17528.725	-23.392219	-131380.86
NiS2(L)										
0	0	0	10.945241	0	0	0	0	-12344.925	-49.720624	0
Ni3S2(I)										
0	0	0	6.92383	0.0404467	-7.31E-05	7.10E-08	-2.62E-11	-29362.196	-32.735052	-216325.16
Ni3S2(II)										
0	0	0	22.685585	0	0	0	0	-29313.479	-111.68978	0
1	0	0	22.685585	0	0	0	0	-29313.479	-111.68978	0
Ni3S2(L)										
0	0	0	23.068039	0	0	0	0	-27344.402	-112.11811	0
Ni3S4(s)										
0	0	0	14.671193	0.0172772	-2.76E-09	1.02E-11	-6.30E-15	-41358.479	-66.312939	-301121.26
1	0	0	14.673818	0.0172757	0	0	0	-41360.001	-66.329162	-301121.26
P(cr)										
0	-5183070.13	123770.23	-1223.2766	6.4367367	-0.0189019	2.95E-05	-1.91E-08	-526197.6	6058.9634	0
P(L)										
0	0	0	3.141496	0	0	0	0	-862.14329	-12.72273	0
P4O10(cr)										
0	-29104.75984	5.2096121	0.0705841	0	0	0	0	-366817.85	-23.107863	-3010100
1	5.461897334	0.0807817	-4.07E-05	0	0	0	0	-366888.92	-25.61194	-3010100
P4O10(L)										
0	44.50051777	0	0	0	0	0	0	-376552.39	-231.17046	-3010100
Pb(cr)										
0	-614963.371	10657.117	-71.298537	0.266839	-5.18E-04	5.24E-07	-2.15E-10	-49740.484	385.58021	0

Pb(L)										
0	-37981.7933	0	4.3642981	-0.0012364	4.95E-07	-5.23E-11	0	-888.73305	-16.195597	0
PbBr2(s)										
0	0	0	6.5657173	0.0195961	-3.19E-05	0	0	-35825.763	-22.457076	-276700
1	80461.747	0	6.8992641	0.0059259	0	0	0	-35329.704	-21.247693	-276700
PbBr2(L)										
0	0	0	13.470427	0	0	0	0	-36480.364	-56.958426	-276700
PbCL2(cr)										
0	2697281.121	-42129.424	265.16419	-0.789135	0.0013169	-1.12E-06	3.85E-10	152276.68	-1434.6618	-359400
PbCL2(L)										
0	0	0	13.350155	0	0	0	0	-46136.902	-59.534196	-359400
PbF2(II)										
0	13638.8073	0	7.1040867	0.0048068	0	0	0	-83589.633	-29.083851	-676000
PbF2(I)										
0	-7.86E+07	0	1154.0135	-2.4130804	0.0014534	0	0	-572048.73	-6285.5796	-676000
1	3.52E+07	0	-158.09254	0.1905777	-5.65E-05	0	0	43707.238	973.59363	-676000
PbF2(L)										
0	0	0	13.109612	0	0	0	0	-84589.5	-62.827757	-676000
PbI2(s)										
0	-6615.8574	0	8.8796587	0.0017583	0	0	0	-23915.625	-30.124664	-176000
1	44284.0288	0	7.7310629	0.0036901	0	0	0	-23488.312	-23.870082	-176000
PbI2(L)										
0	0	0	13.109612	0	0	0	0	-23551.656	-52.379731	-176000
PbO(II-r)										
0	0	0	0.8050625	0.0288498	-4.30E-05	0	0	-27433.619	-3.1170858	-218600
1	-6651.023332	0	4.9395575	0.0024066	0	0	0	-27893.391	-20.739325	-218600
PbO(I-y)										
0	-33603.9045	0	5.4074143	0.0015956	0	0	0	-28025.766	-23.217664	-218600
PbO(L)										
0	0	0	7.8176585	0	0	0	0	-26642.581	-35.709138	-218600
PbO2(s)										
0	0	0	0.100753	0.0403553	-5.40E-05	0	0	-34541.991	-1.5578035	-276000
1	-259305.72	0	10.104023	5.00E-04	0	0	0	-37099.449	-50.526403	-276000
PbS(cr)										
0	-11101.9613	0	5.7885527	9.72E-04	0	0	0	-13770.275	-22.364173	-99474.8
1	-75290.0652	0	7.331761	-0.0022623	1.61E-06	0	0	-14316.154	-30.625143	-99474.8
PbS(L)										
0	0	0	8.0582019	0	0	0	0	-10072.411	-33.165742	-99474.8
Pb2O3(s)										
0	0	0	1.5749674	0.0663369	-9.45E-05	0	0	-61720.8	-6.2826422	-491700
1	-331468.721	0	15.059216	0.0054435	0	0	0	-64981.182	-71.019466	-491700
Pb3O4(cr)										
0	7031601.47	-87704.16	419.58865	-0.9058738	0.0011383	-7.36E-07	1.92E-10	343161.13	-2394.2294	-720000
Rb(cr)										
0	-169367.859	5116.7639	-56.8676	0.3403543	-9.35E-04	1.02E-06	0	-21645.471	280.53507	0
Rb(L)										
0	23623.9429	286.93505	1.5449886	0.0051683	-6.07E-06	3.35E-09	-5.19E-13	-1935.501	1.0695596	0
1	-367448.669	1779.7887	-0.3426047	0.0053231	-4.26E-06	1.70E-09	-4.42E-14	-11113.307	14.779055	0
RbOH(b)										
0	0	0	6.5899253	0.0057313	0	0	0	-52589.299	-27.949989	-418800
RbOH(c)										
0	0	0	9.1406469	0	0	0	0	-52484.05	-39.628555	-418800
RbOH(L)										
0	0	0	10.343364	0	0	0	0	-52313.264	-45.97096	-418800
S(cr1)										
0	-10357.1077	0	1.8667669	0.0042561	-3.27E-06	0	0	-751.63896	-7.961067	0
S(cr2)										
0	0	0	2.0805141	0.0024409	0	0	0	-685.27147	-8.6078468	0
S(L)										
0	-6.37E+07	0	2376.8607	-7.888076	0.0073761	0	0	-635659.49	-11869.296	0
1	0	0	6928.5223	-32.54656	0.0382445	0	0	-983222.27	-31548.068	0
2	0	0	164.99457	-0.6843535	7.32E-04	0	0	-26388.469	-768.17301	0
3	1972984.58	0	-24.410098	0.0609035	-3.74E-05	0	0	11130.134	136.31742	0
4	0	0	3.8486934	0	0	0	0	-828.45898	-17.361282	0
SCL2(L)										
0	0	0	10.945241	0	0	0	0	-9251.7543	-40.269795	-49790.867
1	0	0	10.945241	0	0	0	0	-9251.7543	-40.269795	-49790.867
S2CL2(L)										
0	0	0	14.948935	0	0	0	0	-11451.915	-58.250225	-58159.083
1	0	0	14.948935	0	0	0	0	-11451.915	-58.250225	-58159.083
Sc(a)										
0	-5723.53769	0	1.8350723	0.0094789	-2.32E-05	2.00E-08	0	-822.5089	-8.2791214	0
1	-22964.09436	0	3.5902969	-0.0014802	2.13E-06	-4.65E-10	0	-1099.5438	-16.052554	0
Sc(b)										
0	0	0	5.3160078	0	0	0	0	-3113.44	-28.756865	0
Sc(l)										
0	0	0	5.2919535	0	0	0	0	-1373.9748	-27.641522	0
Si(cr)										
0	-23235.3821	0	2.1020217	0.0018092	0	0	0	-785.06352	-10.384273	0
1	-52325.5973	0	2.8501694	3.98E-04	0	0	0	-1042.9472	-14.389642	0
Si(L)										
0	0	0	3.2713894	0	0	0	0	4882.6671	-13.266111	0

SiC(b)										
0	-2285.49638	0	-0.5349101	0.0127155	0	0	0	-9193.1749	1.2414414	-73000
SiC(b)										
0	-2285.49638	0	-0.5349101	0.0127155	0	0	0	-9193.1749	1.2414414	-73000
SiC(L)										
0	0	0	7.5771152	0	0	0	0	-7787.459	-43.675962	-73000
SiO2(a-qz)										
0	-577689.55	7214.6611	-31.457303	0.0741218	-8.67E-06	-1.08E-07	8.32E-11	-146239.84	184.24244	-910700
SiO2(b-qz)										
0	23176.35074	0	7.0265115	0.0012419	0	0	0	-111701.25	-35.807514	-910700
SiO2(b-crt)										
0	-535641.9079	0	9.3310369	-7.31E-04	3.34E-07	0	0	-113432.67	-49.987684	-910700
SiO2(L)										
0	0	0	10.042684	0	0	0	0	-114000.3	-55.542796	-910700
SiS(cr)										
0	0	0	4.8734081	0.0018072	0	0	0	-21827.637	-20.728416	-168737.21
SiS(L)										
0	0	0	8.0582019	0	0	0	0	-20761.407	-38.515816	-168737.21
SiS2(cr)										
0	-14896.79569	0	3.9217105	0.0122697	0	0	0	-36282.539	-16.842247	-287000
1	0	0	6.4233491	0.0033172	0	0	0	-36580.53	-28.342599	-287000
SiS2(L)										
0	0	0	12.027167	0	0	0	0	-39092.608	-62.76639	-287000
Si2N2O(s)										
0	-7783291.74	77876.963	-322.67266	0.7513787	-9.14E-04	5.77E-07	-1.48E-10	-513986.47	1873.1241	-947700
1	-7408337.81	25572.722	-25.322535	0.0320626	-1.34E-05	3.07E-09	-2.89E-13	-276133.32	190.553	-947700
Si3N4(cr)										
0	-11364.3451	0	-0.4993436	0.0396232	0	0	0	-96400.379	-1.086769	-787800
1	-291045.413	0	11.892102	0.0093498	-2.55E-06	2.86E-10	0	-99665.417	-64.12448	-787800
Sn(cr)										
0	-997024.407	18649.939	-139.29561	0.56526	-0.0012291	1.40E-06	-6.47E-10	-84795.676	731.77269	0
Sn(L)										
0	98478.4431	0	3.0289217	2.53E-04	-1.96E-08	0	0	220.96517	-9.0897838	0
SnBr2(cr)										
0	-10721.4207	0	8.6503887	0.0032469	0	0	0	-33260.284	-31.913241	-253600
1	159636.587	0	4.3106569	0.0113747	0	0	0	-31756.262	-8.652274	-253600
SnBr2(L)										
0	280449.479	0	14.27733	-0.0022182	0	0	0	-33051.622	-60.082382	-253600
1	0	0	12.748797	0	0	0	0	-32883.467	-51.851412	-253600
SnBr4(cr)										
0	-3870038.96	0	366.33303	-1.7756586	0.0025047	0	0	-112073.04	-1659.6262	-388000
SnBr4(L)										
0	112478.0655	0	18.598691	-4.79E-04	0	0	0	-50365.693	-69.136686	-388000
1	0	0	18.882652	0	0	0	0	-50791.407	-71.363678	-388000
SnCL2(cr)										
0	-345565.927	5121.0492	-21.7994	0.0873827	-1.09E-04	5.70E-08	0	-66923.532	133.84123	-333000
SnCL2(L)										
0	0	0	13.229884	0	0	0	0	-42942.404	-57.66925	-333000
SnCL4(L)										
0	0	0	20.59051	-0.005567	0	0	0	-68072.078	-83.784623	-517000
1	0	0	18.642109	0	0	0	0	-67731.118	-74.319475	-517000
SnF2(cr)										
0	0	0	6.5752522	0.0071502	0	0	0	-83702.133	-28.024818	-677000
SnF2(L)										
0	0	0	12.027167	0	0	0	0	-84248.824	-55.698668	-677000
SnI2(cr)										
0	828271.391	-12997.636	84.104459	-0.1990006	2.43E-04	-1.02E-07	0	40253.305	-448.44197	-153000
SnI2(L)										
0	380768.079	0	13.137996	-7.11E-04	0	0	0	-20139.814	-51.934308	-153000
1	0	0	12.869069	0	0	0	0	-20605.706	-50.976324	-153000
SnI4(cr)										
0	1365815.91	-21864.415	141.17687	-0.315197	2.99E-04	0	0	73474.221	-755.33825	-207500
SnI4(L)										
0	312549.988	0	21.145684	-0.0059183	0	0	0	-28286.789	-79.279007	-207500
1	0	0	18.642109	0	0	0	0	-28369.057	-67.24587	-207500
SnO(cr)										
0	0	0	0.0727947	0.0330769	-4.71E-05	0	0	-34837.132	-1.3068287	-280710
1	0	0	5.2606828	0.0016309	0	0	0	-35402.42	-23.583566	-280710
SnO(L)										
0	0	0	7.5771152	0	0	0	0	-33692.308	-35.397986	-280710
SnO2(cr)										
0	0	0	-1.177648	0.0397017	-4.79E-05	0	0	-70462.777	2.896557	-577630
1	-267460.139	0	9.1454578	8.86E-04	0	0	0	-73135.674	-47.981068	-577630
SnO2(L)										
0	0	0	11.064994	0	0	0	0	-72229.941	-59.274559	-577630
SnS(rh)										
0	-14734.90121	0	5.3173164	0.0025867	0	0	0	-14938.981	-21.889107	-109662
1	30561.03126	0	4.5117511	0.0035794	0	0	0	-14591.001	-17.340523	-109662
SnS(cu)										
0	0	0	4.9215167	0.0018823	0	0	0	-14254.199	-18.559221	-109662
SnS(L)										
0	0	0	9.0083481	0	0	0	0	-13916.505	-41.909907	-109662

SnS2(cr)										
0	-28179.80768	0	6.5863397	0.0072597	0	0	0	-19439.875	-29.337544	-141837
1	11930.94963	0	7.5602772	0.0024796	0	0	0	-19383.265	-33.235863	-141837
Sr(a)										
0	-4150.24567	155.98234	-0.2623173	0.0294537	-1.21E-04	2.40E-07	-1.71E-10	-1455.7911	3.4351061	0
1	129441.2876	-1646.1792	11.111142	-0.0197374	2.91E-05	-2.16E-08	6.51E-12	7160.398	-56.716022	0
Sr(b)										
0	0	0	3.1903263	4.84E-04	0	0	0	-856.09913	-11.572384	0
Sr(L)										
0	0	0	4.4500518	0	0	0	0	-943.19404	-18.897034	0
SrBr2(a)										
0	-156386.2878	2048.3873	-2.389925	0.03201	-4.32E-05	3.25E-08	-9.79E-12	-99419.223	28.970075	-722000
SrBr2(b)										
0	0	0	12.027167	0	0	0	0	-90216.505	-52.126639	-722000
SrBr2(L)										
0	0	0	12.027167	0	0	0	0	-89001.761	-50.820463	-722000
SrCO3(a)										
0	-3.19E+07	598394.43	-4555.7787	18.074229	-0.0392255	4.44E-05	-2.06E-08	-2840270.2	23799.27	-1226000
1	-473774.1611	0	18.292479	-0.0134283	1.07E-05	0	0	-153993.98	-91.671972	-1226000
SrCO3(b)										
0	0	0	17.559664	0	0	0	0	-154196.26	-93.02016	-1226000
SrCO3(c)										
0	0	0	17.559664	0	0	0	0	-154196.26	-93.02016	-1226000
SrCO3(L)										
0	0	0	19.844825	0	0	0	0	-153423.27	-107.38378	-1226000
SrCL2(a)										
0	-821930.256	14146.272	-90.668689	0.3537351	-6.60E-04	6.29E-07	-2.41E-10	-167529.99	492.02198	-833000
1	1.11E+09	0	-17187.73	42.548191	-0.0393556	1.29E-05	0	6824931.4	92137.916	-833000
SrCL2(b)										
0	2.65E+08	0	-613.75932	0.3705889	0	0	0	601393.88	4028.3669	-833000
SrCL2(L)										
0	-1621863.465	0	12.784638	0	0	0	0	-104051.82	-60.105009	-833000
SrF2(a)										
0	-14361.81472	-390.27046	9.0845289	0.004747	-9.92E-06	1.17E-08	-4.83E-12	-148491.15	-44.339887	-1229000
1	-1.71E+07	25766.305	32.578934	-0.0303228	-2.83E-05	2.98E-08	-2.38E-12	-351104.38	-151.4197	-1229000
SrF2(b)										
0	5.27E+09	-92870.06	-11883.696	9.8292407	-0.0022773	0	0	1.34E+07	75862.988	-1229000
SrF2(L)										
0	0	0	11.906895	0	0	0	0	-147887.76	-57.967187	-1229000
SrH2(a)										
0	0	0	4.1254385	0.0039124	0	0	0	-23052.795	-18.417451	-180000
SrH2(b)										
0	0	0	8.5392885	0	0	0	0	-24676.6	-44.257957	-180000
SrH2(L)										
0	0	0	9.0203752	0	0	0	0	-22546.83	-45.624953	-180000
SrI2(cr)										
0	-853183.659	13962.949	-81.343812	0.292362	-4.94E-04	4.28E-07	-1.48E-10	-135883.57	455.93769	-568000
SrI2(L)										
0	0	0	13.229884	0	0	0	0	-71430.409	-56.469697	-568000
SrO(cr)										
0	-1625438.799	29323.751	-213.66433	0.8526582	-0.0018196	2.04E-06	-9.34E-10	-205307	1123.7843	-591000
1	-34109.04551	0	5.0492452	0.0034315	-3.04E-06	9.07E-10	0	-72827.82	-23.171637	-591000
2	-3.97E+07	0	78.507332	-0.0533679	1.13E-05	0	0	-160489.69	-499.0589	-591000
SrO(L)										
0	0	0	10.10282	0	0	0	0	-71882.033	-55.415561	-591000
Sr(OH)2(b)										
0	574977.465	-9564.7824	63.104666	-0.1470271	2.47E-04	-2.04E-07	6.87E-11	-73642.792	-342.43402	-964300
Sr(OH)2(a)										
0	0	0	15.635317	0	0	0	0	-121657.65	-80.067374	-964300
Sr(OH)2(L)										
0	0	0	18.401565	0	0	0	0	-121126.53	-95.162621	-964300
SrS(cr)										
0	2688173.776	-50108.467	381.30268	-1.4626232	0.0031389	-3.52E-06	1.62E-09	166572.48	-1992.7607	-480000
1	-12219.60164	0	5.7168733	9.32E-04	0	0	0	-59517.281	-24.71634	-480000
SrS(L)										
0	0	0	8.0582019	0	0	0	0	-54877.273	-37.674118	-480000
SrS04(a)										
0	-252486.3161	0	13.19272	0.0064241	0	0	0	-180301.6	-63.949424	-1457000
SrS04(b)										
0	0	0	20.446184	0	0	0	0	-182726.49	-106.55974	-1457000
SrS04(L)										
0	0	0	20.446184	0	0	0	0	-178396.71	-104.25667	-1457000
Ta(cr)										
0	15199.4043	-492.71415	6.8556044	-0.0136663	2.56E-05	-2.24E-08	7.39E-12	1236.0768	-32.520748	0
1	-1.00E+08	469301.5	-898.62958	0.9078787	-5.04E-04	1.46E-07	-1.73E-11	-2760103.5	5935.3009	0
2	128624.807	562.48159	-2.2640867	0.0067917	-2.95E-06	5.06E-10	-8.39E-15	-1570.9676	19.799829	0
Ta(L)										
0	0	0	5.0321667	0	0	0	0	-743.60421	-25.973627	0
TaC(s)										
0	0	0	1.0249717	0.0176286	-2.55E-05	1.73E-08	-4.31E-12	-18226.597	-5.0093127	-144096.4
1	0	0	5.0027056	0.0012849	-1.75E-07	3.52E-11	-2.64E-15	-19020.553	-24.129691	-144096.4
TaC(L)										

0	0	0	8.0516715	0	0	0	0	-10103.338	-42.085545	0
Ta2O5(s)										
0	0	0	10.119942	0.0255376	-1.68E-05	3.47E-11	3.13E-12	-250081.74	-47.310877	-2046007.3
1	0	0	18.473684	0.0034902	9.12E-07	-1.15E-09	2.47E-13	-252459.11	-90.733491	-2046007.3
Ta2O5(L)										
0	0	0	29.187309	0	0	0	0	-253362.45	-158.57774	0
Th(a)										
0	-14532.4716	150.52224	2.2706948	0.0020586	-9.22E-07	4.32E-10	-7.95E-14	-1667.5364	-6.857177	0
Th(b)										
0	-4483571.08	11999.599	-10.990366	0.0083677	-1.87E-06	2.03E-10	0	-76796.267	89.080507	0
Th(L)										
0	0	0	5.5324968	0	0	0	0	-2191.8251	-27.600719	0
Ti(a)										
0	35985.9866	-827.2302	7.6890954	-0.0114397	1.39E-05	-4.69E-09	-9.85E-13	2936.6195	-39.851367	0
1	-2876235.71	0	45.731532	-0.0769238	3.80E-05	0	0	-20380.239	-251.62702	0
Ti(b)										
0	-1625891.9	6281.0783	-8.0601507	0.0093486	-3.77E-06	1.07E-09	-1.14E-13	-37520.337	61.729429	0
Ti(L)										
0	0	0	5.6287141	0	0	0	0	-2377.3547	-30.794435	0
TiB(cr)										
0	589296.246	-7628.3872	32.645042	-0.0443868	4.04E-05	-1.90E-08	3.66E-12	18085.665	-192.49267	-160247
1	973623.896	-2744.3062	9.195602	-0.0016367	5.68E-07	-9.26E-11	6.11E-15	-3925.0823	-53.674246	-160247
TiB2(cr)										
0	270188.5716	-3989.107	19.045958	-0.0146795	1.25E-05	-4.48E-09	5.93E-13	-15108.187	-113.09013	-279491
1	2.45E+10	-5.42E+07	49843.86	-24.373149	0.0066885	-9.76E-07	5.92E-11	3.59E+08	-365140.63	-279491
TiB2(L)										
0	0	0	13.083633	0	0	0	0	-32981.723	-76.491311	-279491
TiC(s)										
0	0	0	-1.3633942	0.0282522	-4.12E-05	2.68E-08	-6.35E-12	-22678.352	3.8626483	-184107.87
1	0	0	5.9413936	-3.73E-04	7.12E-07	-1.35E-10	9.98E-15	-24173.445	-31.530222	-184107.87
TiC(L)										
0	0	0	7.5484421	0	0	0	0	-17660.204	-40.629661	0
TiCL2(s)										
0	0	0	5.7567518	0.013631	-2.04E-05	1.59E-08	-4.55E-12	-64169.918	-25.585456	-515489.37
1	0	0	7.9684147	0.0025448	-2.86E-07	1.32E-10	-2.23E-14	-64508.442	-35.713089	-515489.37
TiCL3(s)										
0	0	0	10.937936	0.0026623	-1.48E-07	-1.54E-09	9.22E-13	-90182.668	-46.287287	-721758.57
1	0	0	11.462658	0.0014018	-3.07E-08	1.23E-13	-1.06E-17	-90316.96	-48.993078	-721758.57
TiCL4(L)										
0	0	0	17.066042	0.0015777	-1.09E-06	1.04E-09	-3.60E-13	-101871.34	-67.308228	-804185.19
1	0	0	17.142643	0.0010937	-1.07E-09	2.66E-13	-2.28E-17	-101880.27	-67.640142	-804185.19
TiN(s)										
0	0	0	-2.5320119	0.0411749	-7.71E-05	6.53E-08	-2.06E-11	-41124.666	8.6750796	-337660.38
1	0	0	5.6010051	3.56E-04	3.95E-07	-8.87E-11	7.78E-15	-42443.43	-28.773293	-337660.38
TiN(L)										
0	0	0	7.5484421	0	0	0	0	-36261.709	-39.583906	0
TiO(a)										
0	0	0	0.8980956	0.0213544	-3.58E-05	3.04E-08	-9.71E-12	-66224.332	-5.9567004	-542676.36
1	0	0	2.6516785	0.0079963	-4.96E-06	1.41E-09	0	-66288.361	-12.918703	-542676.36
TiO(b)										
0	0	0	1.7971419	0.0101289	-7.46E-06	3.08E-09	-4.76E-13	-65482.773	-7.9349175	0
TiO(L)										
0	0	0	8.0516715	0	0	0	0	-63272.138	-41.312109	0
TiO2(ru)										
0	0	0	-0.1611752	0.0379667	-6.52E-05	5.26E-08	-1.62E-11	-114788.97	-1.8874035	-944769.12
1	0	0	6.8489151	0.0042463	-3.01E-06	1.06E-09	-1.44E-13	-115992.46	-34.514106	-944769.12
TiO2(L)										
0	0	0	12.077507	0	0	0	0	-114942.3	-65.910759	0
Ti2O3(a)										
0	0	0	14.623542	-0.0371617	9.00E-05	0	0	-186416.93	-66.914899	-1520834.4
Ti2O3(b)										
0	0	0	1.6977485	0.0571374	-8.33E-05	5.73E-08	-1.52E-11	-185250.36	-14.066559	0
1	0	0	14.874222	0.0045466	-2.36E-06	6.00E-10	-5.34E-14	-187973.42	-77.863165	0
Ti2O3(L)										
0	0	0	18.871105	0	0	0	0	-178586.98	-96.567257	0
Ti3O5(a)										
0	0	0	-3.7337434	0.1061932	-1.05E-04	0	0	-298456.17	9.8241016	-2459221.1
Ti3O5(b)										
0	0	0	18.692817	0.0085051	-5.12E-06	4.61E-09	-1.52E-12	-300128.95	-89.889586	0
1	0	0	18.415159	0.0080013	-1.99E-06	8.78E-10	-1.42E-13	-299986.84	-88.135479	0
Ti3O5(L)										
0	0	0	32.206686	0	0	0	0	-293685.41	-169.12703	0
Ti4O7(s)										
0	0	0	-0.8633356	0.1416046	-2.32E-04	1.82E-07	-5.48E-11	-413794.84	-4.563758	-3404610
1	0	0	24.112915	0.0229277	-1.71E-05	6.48E-09	-9.49E-13	-418107.16	-121.0465	-3404610
Ti4O7(L)										
0	0	0	44.284194	0	0	0	0	-410896.73	-235.16043	0
U(a)										
0	-15408.9926	231.88017	1.2279447	0.0071361	-1.02E-05	1.14E-08	-3.67E-12	-1986.9217	-2.0359751	0
U(b)										
0	0	0	5.0995188	0	0	0	0	-1672.0802	-23.780301	0
U(c)										

0	0	0	4.606405	0	0	0	0	-585.91873	-19.80809	0
U(L)										
0	-94645.7587	852.60938	4.2091845	8.41E-04	-1.31E-07	1.98E-11	-1.23E-15	-5956.0586	-16.672882	0
V(cr)										
0	284512.855	-5094.9378	37.150224	-0.1176032	2.26E-04	-2.26E-07	9.29E-11	22543.804	-196.82436	0
1	1371659.69	-7844.9858	20.944618	-0.020547	1.32E-05	-4.04E-09	5.08E-13	43733.729	-129.23365	0
2	3.01E+08	-1125907.3	1747.4386	-1.4330396	6.59E-04	-1.61E-07	1.63E-11	6867132.4	-11885.898	0
V(L)										
0	0	0	5.5570322	0	0	0	0	-1899.6667	-30.705302	0
VCL2(s)										
0	0	0	6.7395599	0.0104872	-1.72E-05	1.48E-08	-4.76E-12	-56698.886	-29.205704	-451882.13
1	0	0	6.2711216	0.007489	-5.25E-06	1.51E-09	0	-56358.056	-25.726538	-451882.13
VCL3(s)										
0	0	0	6.9770413	0.023542	-4.07E-05	3.49E-08	-1.12E-11	-72678.169	-29.493712	-580750.74
VCL4(L)										
0	0	0	17.462063	0	0	0	0	-73695.845	-68.794792	-569456.89
1	0	0	17.462063	0	0	0	0	-73695.845	-68.794792	-569456.89
VN(s)										
0	0	0	0.8127136	0.020101	-3.12E-05	2.31E-08	-6.38E-12	-27020.094	-4.9457436	-217151.45
1	0	0	4.836874	0.00189	-3.16E-07	4.61E-11	-1.91E-15	-27738.152	-23.873353	-217151.45
VO(s)										
0	0	0	2.5380401	0.0164471	-2.86E-05	2.48E-08	-7.99E-12	-53211.919	-13.599758	-431782.45
1	0	0	5.3398715	0.0017592	3.85E-07	-2.62E-10	5.10E-14	-53651.379	-26.382364	-431782.45
VO(L)										
0	0	0	7.5484421	0	0	0	0	-47600.474	-36.154213	0
V2O3(s)										
0	0	0	2.2877033	0.0576328	-9.67E-05	7.41E-08	-2.07E-11	-149111.89	-14.723446	-1218793.1
1	0	0	13.964211	0.0016871	1.14E-06	-2.08E-10	1.00E-14	-151005.75	-68.782894	-1218793.1
V2O3(L)										
0	0	0	18.871105	0	0	0	0	-140340.63	-94.58092	0
V2O4(I)										
0	0	0	6.8914542	0.0099142	5.78E-05	4.31E-08	-2.85E-10	-174608.64	-32.157358	-1427198.1
V2O4(II)										
0	0	0	4.9003624	0.050027	-7.13E-05	4.65E-08	-1.08E-11	-173736.76	-24.503375	0
1	0	0	16.610256	0.0023329	9.89E-07	-7.50E-10	1.61E-13	-176073.89	-80.831997	0
V2O4(L)										
0	0	0	25.664703	0	0	0	0	-174630.09	-136.5594	0
V2O5(s)										
0	0	0	-1.164036	0.0935359	-1.57E-04	1.22E-07	-3.57E-11	-189145.31	0.4072275	-1550616.1
V2O5(L)										
0	0	0	22.947264	0	0	0	0	-187514.47	-110.89277	0
1	0	0	22.947264	0	0	0	0	-187514.47	-110.89277	0
W(cr)										
0	-6824.55464	-225.42472	4.9766035	-0.0069264	1.20E-05	-9.34E-09	2.82E-12	-3.5115698	-23.613344	0
1	552886.294	-2041.0002	5.8700857	-0.0019201	1.07E-06	-2.35E-10	2.16E-14	11635.171	-33.186584	0
2	1.92E+10	-3.04E+07	17813.399	-4.2385766	5.06E-05	1.40E-07	-1.66E-11	2.13E+08	-140097.69	0
3	3.79E+10	-6.90E+07	48176.329	-16.344312	0.0027117	-1.77E-07	0	4.73E+08	-368164.87	0
W(L)										
0	0	0	4.2773417	0	0	0	0	2755.4149	-20.864489	0
WC(cr)										
0	-111975.4391	-0.5553268	5.2179652	0.0010379	-1.23E-07	2.88E-13	-7.24E-17	-6848.9987	-26.770662	-40540
WCL6(I)										
0	166.1826519	0	15.088731	0.0201565	-2.75E-08	0	0	-76800.288	-63.293659	-593710
WCL6(II)										
0	-9897.04636	0	15.22858	0.0199438	0	0	0	-76361.662	-62.96167	-593710
WCL6(III)										
0	0	0	22.64475	0	0	0	0	-75652.178	-95.271654	-593710
WCL6(L)										
0	0	0	24.1544	0	0	0	0	-75684.936	-103.36046	-593710
WOCL4(cr)										
0	1295.153216	0	13.785221	0.0127618	-1.71E-07	0	0	-85387.427	-61.549838	-671114
WOCL4(L)										
0	0	0	21.889925	0	0	0	0	-82366.563	-94.223214	-671114
WO2(cr)										
0	-17338.42408	0	2.5589798	0.0145726	0	0	0	-72200.586	-12.931823	-588100
WO2(cr)										
0	-17338.42408	0	2.5589798	0.0145726	0	0	0	-72200.586	-12.931823	-588100
WO2CL2(cr)										
0	-381941.002	2367.0297	9.8344558	-0.0250844	1.02E-04	-1.04E-07	3.47E-11	-111144.04	-22.279299	-780316
WO3(crIII)										
0	-284114.0443	7257.7148	-67.084051	0.3092936	-4.13E-04	0	0	-133588.42	340.91137	-841300
WO3(crIII,II)										
0	-51861.14395	0	8.5483089	0.0043172	0	0	0	-104093.52	-40.446707	-841300
WO3(crI)										
0	0	0	9.7375552	0.0019586	0	0	0	-103916.63	-46.143904	-841300
WO3(L)										
0	0	0	15.515045	0	0	0	0	-102241.21	-80.829275	-841300
Zn(cr)										
0	370205.418	-5915.4318	39.594711	-0.1143726	1.93E-04	-1.68E-07	6.08E-11	26817.17	-211.48325	0
Zn(L)										
0	0	0	3.7765304	0	0	0	0	-431.73458	-15.670779	0
ZnSO4(a)										

0	0	0	5.1657364	0.0239774	-3.07E-06	-4.85E-09	0	-120453.59	-23.105369	-980151.05
ZnSO4(a)										
0	0	0	5.1657364	0.0239774	-3.07E-06	-4.85E-09	0	-120453.59	-23.105369	-980151.05
ZnSO4(b)										
0	0	0	17.461825	0	0	0	0	-121138.06	-85.143253	0
Zr(a)										
0	-11536.9959	26.262086	2.9320544	5.74E-04	-7.65E-07	1.60E-09	-6.10E-13	-1084.1535	-12.157768	0
Zr(b)										
0	-1062988.7	4263.2634	-3.1580584	0.0050053	-2.36E-06	7.69E-10	-8.14E-14	-26353.552	30.613596	0
Zr(L)										
0	0	0	5.0321667	0	0	0	0	-1100.7959	-25.48066	0
ZrN(s)										
0	0	0	2.855629	0.0086167	-5.35E-06	-2.88E-09	3.11E-12	-45112.02	-13.901069	-365249.01
1	0	0	5.540782	6.18E-04	2.95E-07	-1.18E-10	1.52E-14	-45751.324	-27.420654	-365249.01
ZrN(L)										
0	0	0	7.0451164	0	0	0	0	-38105.527	-34.436264	0
ZrO2(a)										
0	0	0	-0.7953711	0.0439335	-8.12E-05	6.96E-08	-2.24E-11	-133119.67	0.5322101	-1097471.4
1	0	0	-22.144395	0.0996398	-1.20E-04	6.47E-08	-1.30E-11	-127327.97	111.00891	-1097471.4
ZrO2(b)										
0	0	0	8.9573629	0	0	0	0	-134143.54	-45.274017	0
ZrO2(L)										
0	0	0	10.567675	0	0	0	0	-128427.45	-54.592264	0
Air										
0	10099.5016	-196.82756	5.0091551	-0.005761	1.07E-05	-7.94E-09	2.19E-12	-176.79673	-3.921501	-125.53
1	241521.443	-1257.8746	5.1445587	-2.14E-04	7.07E-08	-1.07E-11	6.58E-16	6462.2632	-8.1474087	-125.53
B2H6(L)										
B5H9(L)										
(CH2)x(s)										
CH3NO2(L)										
CH4(L)										
CH3OH(L)										
0	-1302005.2	31669.85	-303.124	1.602232	-0.00459	6.99E-06	-4.21E-09	-165617	1514.347	-238910
CH6N2(L)										
C2H2(L),acetyle										
CH3CN(L)										
C2H4(L)										
C2H4O(L),ethyle										
C2H6(L)										
C2H5OH(L)										
0	450111.594	-10208.3	101.4267	-0.38747	7.12E-04	-1.86E-07	-2.04E-10	7448.558	-504.426	-277510
C2H8N2(L),UDMH										
C2N2(L)										
C3H6(L),propyle										
C3H7NO3(L)										
C3H8(L)										
C4H8(L),1-buten										
C4H10(L),n-buta										
C4H10(L),isobut										
C5H12(L),n-pent										
C6H6(L)										
0	-2560137.1	41367.46	-212.297	0.372358	7.56E-04	-3.08E-06	2.79E-09	-193547	1231.846	49080
C6H5NH2(L)										
0	6.27E+07	-894751	5067.616	-14.0216	0.018996	-9.32E-06	-1.24E-09	4275411	-28077.7	31500
C6H14(L),n-hexa										
0	7730917.16	-225189	2719.903	-16.9987	0.059124	-1.08E-04	8.03E-08	881946.6	-12941.4	-198660
C7H8(L)										
0	-3713560	77725.51	-631.229	2.7244	-0.0061	7.02E-06	-3.11E-09	-345213	3265.99	12180
C7H16(L),n-hept										
0	1760036	-37496	396.326	-2.11792	0.006829	-1.13E-05	7.74E-09	126916	-1921.78	-224350
C8H18(L),n-octa										
0	-2.32E+07	484653.5	-4084.82	18.20819	-0.04466	5.81E-05	-3.15E-08	-2166270	20916.6	-250260
C8H18(L),isooct										
0	4781047.66	-112691	1096.522	-5.34412	0.0146	-2.03E-05	1.13E-08	443284.9	-5457.91	-259160
CLF3(L)										
CLO3F										
0	44608.777	-589.208	3.558713	0.028096	-3.61E-05	2.27E-08	-5.72E-12	-1388.8	4.591514	-23800
1	-391041.34	-1193.26	13.88663	-3.54E-04	7.83E-08	-8.98E-12	4.16E-16	-1274.85	-51.0649	-23800
CLO3F(L)										
CL2(L)										
F2(L)										
F2O(L)										
HNO3(L)										
H2(L)										
H2O2(L)										
0	0	0	10.74387	0	0	0	0	-25787.9	-48.0322	-187780
IRFNA										
JP-4										
JP-5										
Jet-A(L)										
0	-421846.73	-5576.23	152.2094	-0.86101	0.003072	-4.70E-06	2.74E-09	-32385.4	-678.095	-303403
Jet-A(g)										

0	-606869.93	8328.264	-43.1232	0.257239	-2.63E-04	1.64E-07	-4.65E-11	-76069.7	279.4307	-249657
1	1.54E+07	-74338.7	146.8645	-0.01297	2.16E-06	-1.89E-10	6.60E-15	399632.3	-926.668	-249657
LiCLO4(s)										
NF3(L)										
NH3(L)										
NH4CLO4(I)										
0	-3075.3456	-213.651	10.21583	0.016595	1.67E-05	-2.31E-08	1.54E-11	-38257.7	-42.3025	-295767
NH4CLO4(II)										
0	4.30E+07	-317842	959.1438	-1.43988	0.001223	-5.22E-07	8.80E-11	1687446	-5889.48	-295767
NH4NO3(IV)										
0	-1.63E+07	261460.3	-1680.05	5.448972	-0.00859	5.34E-06	0	-1264195	9085.696	-365600
1	0	0	5.865649	0.03643	0	0	0	-47339.4	-26.1436	-365600
NH4NO3(III)										
0	0	0	7.233138	0.023333	0	0	0	-46941.8	-29.2985	-365600
NH4NO3(II)										
0	0	0	60.23205	-0.1768	0	4.53E-07	0	-54786.3	-275.781	-365600
NH4NO3(I)										
0	0	0	12.95326	0.015635	0	0	0	-47837	-58.4851	-365600
NH4NO3(L)										
0	0	0	19.36374	0	0	0	0	-48437.9	-89.0301	-365600
N2(L)										
N2H4(L)										
0	20809.6574	-741.817	19.16569	-0.04539	1.34E-04	-1.47E-07	6.06E-11	5735.408	-88.2021	50380

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e-              Ref-Species. JANAF 1985 3/82.
 3 g12/98 E   1.00    0.00    0.00    0.00    0.00 0.000548579903         0.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02-1.172081224D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02-1.172081224D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02-1.172081224D+01
Ag              Hf:CODATA1989. Spec:NSRDS-NBS 35 v3 1971.
 3 g10/97 AG  1.00    0.00    0.00    0.00    0.00 0  107.8682000     284900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               3.352002370D+04 6.562819350D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-3.309926370D+05 9.820086420D+02 1.381179917D+00 6.170899990D-04-1.688114600D-07
 2.008826848D-11-5.627285655D-16               2.726719171D+04 1.456862733D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-3.717441500D+08 2.758069172D+05-7.385982610D+01 9.606158720D-03-5.393935740D-07
 1.358856730D-11-1.272610104D-16              -2.107724971D+06 6.628374570D+02
Ag+             Spec: NSRDS-NBS 35 v3 1971.
 3 g10/97 AG  1.00E  -1.00    0.00    0.00    0.00 0  107.8676514    1022093.730
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.530
 3.691132750D+06-4.316983000D+04 2.028445385D+02-4.658413740D-01 5.586200510D-04
-3.154880975D-07 6.578702060D-11               3.371574470D+05-1.142924427D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.530
-5.327432350D+07 1.310710631D+05-1.098820208D+02 4.826002760D-02-1.093661557D-05
 1.263835910D-09-5.852542535D-14              -7.439122510D+05 8.446266190D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.530
-2.119469170D+08 1.159621936D+05-2.220792532D+01 2.938747589D-03-1.822389545D-07
 5.823925360D-12-7.455184012D-17              -8.068014150D+05 2.271702823D+02
Ag-             JPCRD v14 n3 1985 p731.
 3 g10/97 AG  1.00E   1.00    0.00    0.00    0.00 0  107.8687486     153078.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.766565919D+04 5.869679800D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.766565919D+04 5.869679800D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.766565919D+04 5.869679800D+00
AL              Spec:JPCRD v20 n5 p775 1991. Hf:CODATA 1989 p24.
 3 g12/97 AL  1.00    0.00    0.00    0.00    0.00 0   26.9815380     330000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6918.671
```

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 5.006608890D+03 1.861304407D+01 2.412531111D+00 1.987604647D-04-2.432362152D-07
 1.538281506D-10-3.944375734D-14              3.887412680D+04 6.086585765D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6918.671
-2.920820938D+04 1.167751876D+02 2.356906505D+00 7.737231520D-05-1.529455262D-08
-9.971670260D-13 5.053278264D-16              3.823288650D+04 6.600920155D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6918.671
-5.040682320D+08 3.802322650D+05-1.082347159D+02 1.549444292D-02-1.070103856D-06
 3.592110900D-11-4.696039394D-16             -2.901050501D+06 9.491883160D+02
AL+             Spec:JPCRD v20 n5 1991 p775; NSRDS-NBS 35 v1 1971.
 3 g 1/98 AL  1.00E  -1.00    0.00    0.00    0.00 0   26.9809894     913015.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              1.090644788D+05 3.791005785D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-4.181183250D+03-9.948557270D+00 2.548615878D+00-5.878760040D-05 3.132291294D-08
-7.748894630D-12 7.274447690D-16              1.091011485D+05 3.488667295D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-9.334287450D+08 5.671435510D+05-1.320836076D+02 1.565436608D-02-9.324005710D-07
 2.862382268D-11-3.576503634D-16             -4.396182400D+06 1.177085870D+03
AL-             Spec:JANAF 6/83. EA:JPCRD v14 n3 1985 p731.
 3 g 3/97 AL  1.00E   1.00    0.00    0.00    0.00 0   26.9820866     281090.113
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6756.213
 2.910800014D+04-3.836981670D+02 4.655141860D+00-6.045819640D-03 8.577256840D-06
-5.476258170D-09 1.322713578D-12              3.490616880D+04-5.957092275D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6756.213
 6.339829490D+05-2.383442269D+03 5.469974720D+00-1.299842045D-03 2.888309666D-07
-3.253245760D-11 1.472438690D-15              4.780309030D+04-1.536909451D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6756.213
 5.900938300D+06-2.295848307D+03 3.072740558D+00-6.894315690D-05 4.413059860D-09
-1.445270534D-13 1.905642152D-18              5.241748900D+04 1.452081295D+00
ALBO2           JANAF 6/66 JPCRD v14 sup 1 1985.
 2 J 6/66 AL  1.00B   1.00O   2.00    0.00    0.00 0   69.7913380    -541416.208
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.308723400D+00 1.889053900D-02-2.063334800D-05
 1.025132400D-08-1.694128300D-12             -6.648216700D+04 1.447701848D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.172299500D+00 2.978074100D-03-1.243110700D-06
 2.318877900D-10-1.604120800D-14             -6.768368200D+04-9.981739782D+00
ALBr            D0,Props: TPIS 1996 pt1 p184; pt2 p148.
 2 tpis96 AL  1.00BR  1.00    0.00    0.00    0.00 0  106.8855380      14325.015
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9571.115
 8.176158640D+03-2.516942718D+02 5.403296330D+00-1.747212920D-03 2.077304770D-06
-1.261267579D-09 3.166335970D-13              1.635024429D+03-2.323594886D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9571.115
-6.103395600D+05 2.010066834D+03 1.769617961D+00 1.929888914D-03-6.641047830D-07
 1.172854627D-10-7.178742760D-15             -1.217812867D+04 2.204450764D+01
ALBr2           Hf0 & cons: Gurvich TPIS 1996 pt1 p186; pt2 p149.
 2 tpis96 AL  1.00BR  2.00    0.00    0.00    0.00 0  186.7895380    -140662.125
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13397.875
 3.199375870D+04-7.119178970D+02 9.478258110D+00-4.875531670D-03 5.516512990D-06
-3.340053040D-09 8.368476840D-13             -1.540591306D+04-1.742171366D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13397.875
-3.523782900D+05 4.671544170D+02 7.111908190D+00-5.551709200D-04 3.166301130D-07
-5.521028330D-11 3.176725950D-15             -2.265004078D+04-2.695610360D+00
ALBr3           Hf0 & cons: Gurvich TPIS 1996 pt1 p188; pt2 p151.
 2 tpis96 AL  1.00BR  3.00    0.00    0.00    0.00 0  266.6935380    -410476.664
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17943.336
 4.718948840D+04-1.053853163D+03 1.350747168D+01-6.639869930D-03 7.269276830D-06
-4.278049490D-09 1.045573281D-12             -4.699440330D+04-3.667936780D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17943.336
-8.935527440D+04-2.678035134D+01 1.002063997D+01-8.458764400D-06 1.904243317D-09
-2.215195785D-13 1.038219389D-17             -5.249247640D+04-1.579666403D+01
ALC             D0,Props:TPIS 1996 pt1 p205; pt2 p165.
 2 tpis96 AL  1.00C   1.00    0.00    0.00    0.00 0   38.9922380     682283.509
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9058.109
 4.139921880D+04-5.858677890D+02 5.962445720D+00-2.006064322D-03 1.665566136D-06
-7.121649210D-10 1.271188744D-13              8.383436110D+04-8.002165050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9058.109
 1.937001487D+06-6.749117790D+03 1.347525643D+01-5.850802650D-03 1.926461091D-06
-2.585922351D-10 1.222659806D-14              1.225363649D+05-6.152244872D+01
ALC2            Hf0 & cons: Gurvich TPIS 1996 pt1 p206; pt2 p166.
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 2 tpis96 AL  1.00C   2.00    0.00    0.00    0.00 0   51.0029380     675615.776
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12262.776
 1.524087465D+04-2.649987059D+02 6.280414900D+00-1.786037647D-04 3.791907740D-06
-3.999450070D-09 1.299752388D-12                8.092763280D+04-6.247291862D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12262.776
 1.466017895D+05-1.362764489D+03 8.457759150D+00-3.678901680D-04 7.903174500D-08
-8.880023720D-12 4.053633950D-16                8.705924230D+04-2.127956728D+01
ALCL            Hf0,TabData:Gurvich TPIS 1996 pt1 p168; pt2 p131.
 2 tpis96 AL  1.00CL  1.00    0.00    0.00    0.00 0   62.4342380     -51007.443
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9323.112
 2.380881392D+04-4.457159420D+02 5.992853990D+00-2.777300261D-03 3.101582418D-06
-1.815268376D-09 4.414662340D-13               -5.202736030D+03-7.383305224D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9323.112
-8.993461220D+05 2.765942061D+03 1.003500696D+00 2.267806833D-03-7.280541600D-07
 1.182380673D-10-6.660498130D-15               -2.496164448D+04 2.616924759D+01
ALCL+           JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00CL  1.00E  -1.00    0.00    0.00 0   62.4336894     861926.257
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 2.869835200D+00 6.653458600D-03-1.132770700D-05
 9.070297400D-09-2.779464000D-12                1.025974100D+05 1.001995258D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.628496500D+00-3.475053500D-04 2.299735100D-07
-2.427979800D-11-2.644054400D-16                1.022044700D+05 1.430399866D+00
ALCL2           Hf0 & cons: Gurvich TPIS 1996 pt1 p171; pt2 p132.
 2 tpis96 AL  1.00CL  2.00    0.00    0.00    0.00 0   97.8869380    -240874.252
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12846.859
 5.340545950D+04-9.678057980D+02 1.006252671D+01-5.539528450D-03 5.823420560D-06
-3.306542450D-09 7.831562100D-13               -2.607627110D+04-2.393365135D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12846.859
 4.303453060D+05-1.552370585D+03 8.760657420D+00-9.467450060D-04 2.401844880D-07
-2.427836709D-11 8.390123470D-16               -2.145884709D+04-1.803642587D+01
ALCL3           Hf0 & cons: Gurvich TPIS 1996 pt1 p173; pt2 p134.
 2 tpis96 AL  1.00CL  3.00    0.00    0.00    0.00 0  133.3396380    -584678.863
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16400.803
 7.750600970D+04-1.440779717D+03 1.401744141D+01-6.381631240D-03 5.871674720D-06
-2.908872278D-09 5.994050890D-13               -6.579343180D+04-4.494018811D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16400.803
-1.378630916D+05-5.579207290D+01 1.004190387D+01-1.682165339D-05 3.724664660D-09
-4.275526780D-13 1.982341329D-17               -7.343407470D+04-2.045131441D+01
ALCL2+          JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00CL  2.00E  -1.00    0.00    0.00 0   97.8863894     481172.859
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.356112800D+00 1.264061200D-02-2.155406000D-05
 1.722275300D-08-5.274447300D-12                5.616973600D+04 4.493047365D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 7.095457700D+00 4.652547000D-04-2.076647900D-07
 4.087990600D-11-2.956891400D-15                5.564377500D+04-8.518098635D+00
ALCL2-          JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00CL  2.00E   1.00    0.00    0.00 0   97.8874866    -481171.188
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.251094600D+00 1.196856200D-02-2.153822900D-05
 1.786923000D-08-5.622075300D-12               -5.951306100D+04 7.393261835D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 6.712561800D+00 3.465683600D-04-1.588435400D-07
 2.995006300D-11-1.654481500D-15               -5.995425700D+04-4.136329165D+00
ALF             Hf0,Props: TPIS 1996 pt1 p151; pt2 p116.
 2 tpis96 AL  1.00F   1.00    0.00    0.00    0.00 0   45.9799412    -264060.446
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8892.107
 3.020771686D+04-3.080986949D+02 3.886413140D+00 3.564343690D-03-5.858471280D-06
 4.388109920D-09-1.256906273D-12               -3.117572862D+04 2.032567172D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8892.107
-7.111229050D+05 1.903013316D+03 2.191607179D+00 1.421471467D-03-4.179634770D-07
 6.153804400D-11-2.945403999D-15               -4.540728960D+04 1.613163743D+01
ALF+            JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00F   1.00E  -1.00    0.00    0.00 0   45.9793926     692050.575
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 2.725305300D+00 4.812031300D-03-5.441171900D-06
 2.743908400D-09-3.587519200D-13                8.225046800D+04 9.723361057D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 3.352218600D+00 1.310386700D-03-1.431838300D-07
-4.544233000D-11 7.342074900D-15                8.223250000D+04 7.083708357D+00
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ALFCL           Hf0 & cons: Gurvich TPIS 1996 pt1 p182; pt2 p144
 2 tpis96 AL  1.00F   1.00CL  1.00    0.00    0.00 0   81.4326412    -436409.913
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12133.195
 4.104779480D+04-5.769646420D+02 6.562642700D+00 4.106285840D-03-7.213921120D-06
 5.486401450D-09-1.580656193D-12              -5.114828700D+04-6.041232579D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12133.195
 6.970636350D+04-6.224485910D+02 7.573475410D+00-2.236155999D-04 2.382317949D-08
 4.443785760D-12-5.486977850D-16              -5.100943200D+04-1.091165058D+01
ALFCL+          JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00F   1.00CL  1.00E  -1.00    0.00 0   81.4320926     276151.350
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.734129200D+00 1.388904300D-02-2.222253900D-05
 1.693768300D-08-5.006134200D-12              3.164775500D+04 6.669147451D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.883590500D+00 7.050936600D-04-3.136608800D-07
 6.160731000D-11-4.449053700D-15              3.100599000D+04-8.482113549D+00
ALFCL2          Hf0 & cons: Gurvich TPIS 1996 pt1 p183; pt2 p146.
 2 tpis96 AL  1.00F   1.00CL  2.00    0.00    0.00 0  116.8853412    -791395.404
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15738.260
 6.955607340D+04-1.188857902D+03 1.156672590D+01 4.574959490D-04-3.407372830D-06
 3.356822540D-09-1.085329228D-12              -9.162049260D+04-3.206065851D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15738.260
-1.720360526D+05-1.193340759D+02 1.008894431D+01-3.550993810D-05 7.830952610D-09
-8.961734230D-13 4.145330260D-17              -9.804185470D+04-2.127047629D+01
ALF2            Hf0,cons: TPIS 1996 pt1 p153; pt2 p117.
 2 tpis96 AL  1.00F   2.00    0.00    0.00    0.00 0   64.9783444    -631764.175
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11600.932
 2.994951991D+04-2.194199915D+02 3.416748760D+00 1.272953936D-02-1.883312206D-05
 1.330702256D-08-3.680118630D-12              -7.607537650D+04 8.759626916D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11600.932
-2.146896245D+05 3.096840150D+01 6.816399620D+00 1.820129379D-04-7.793677440D-08
 1.472534201D-11-8.803695300D-16              -7.884002680D+04-7.915370474D+00
ALF2+           JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00F   2.00E  -1.00    0.00    0.00 0   64.9777958      92050.255
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.123917600D+00 1.452305600D-02-2.131544300D-05
 1.515613300D-08-4.237409600D-12              9.654507200D+03 7.474176427D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.592539400D+00 1.031948900D-03-4.573944000D-07
 8.962059900D-11-6.460982500D-15              8.899194300D+03-9.459697673D+00
ALF2-           EA,Cons: TPIS 1996 pt1 p154; pt2 p118.
 2 tpis96 AL  1.00F   2.00E   1.00    0.00    0.00 0   64.9788930    -853230.685
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11331.815
 1.233367436D+05-1.348193677D+03 8.611169700D+00 2.245337307D-04-2.424698162D-06
 2.214148816D-09-6.602757380D-13              -9.708438370D+04-2.192612755D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11331.815
-1.590071224D+05-2.060500592D+02 7.155290700D+00-6.260229340D-05 1.391950967D-08
-1.603920201D-12 7.461601850D-17              -1.040479336D+05-1.122697616D+01
ALF2CL          Hf0 & cons: Gurvich TPIS 1996 pt1 p182; pt2 p145.
 2 tpis96 AL  1.00F   2.00CL  1.00    0.00    0.00 0  100.4310444    -999128.145
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14827.517
 5.677412090D+04-8.869829470D+02 8.752746550D+00 8.195791200D-03-1.380480934D-05
 1.032703706D-08-2.948968416D-12              -1.177936778D+05-1.858347808D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14827.517
-2.115422988D+05-1.959188681D+02 1.014576850D+01-5.813219350D-05 1.281071982D-08
-1.465366277D-12 6.776002450D-17              -1.227153110D+05-2.359853846D+01
ALF3            Hf0 & cons: Gurvich TPIS 1996 pt1 p157; pt2 p120.
 2 tpis96 AL  1.00F   3.00    0.00    0.00    0.00 0   83.9767476   -1209276.938
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14043.722
 4.410263520D+04-5.667495740D+02 5.833072850D+00 1.603535069D-02-2.413263602D-05
 1.714106160D-08-4.747543200D-12              -1.443349991D+05-5.461613658D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14043.722
-2.493972160D+05-2.911202519D+02 1.021662932D+01-8.642985970D-05 1.905713108D-08
-2.181058411D-12 1.009055287D-16              -1.475694276D+05-2.703983244D+01
ALF4-           Hf0 & cons: Gurvich TPIS 1996 pt1 p159; pt2 p121.
 2 tpis96 AL  1.00F   4.00E   1.00    0.00    0.00 0  102.9756994   -1951600.806
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16786.835
 2.312010037D+05-3.235376780D+03 2.017865547D+01-9.108193500D-03 6.679552630D-06
-2.606075106D-09 4.110060510D-13              -2.211784563D+05-8.677268282D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16786.835
-3.217411610D+05-2.612097043D+02 1.319792654D+01-8.010135410D-05 1.786204421D-08
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-2.062751964D-12 9.612581770D-17              -2.381577915D+05-4.231634322D+01
ALH            D0 TabData:Gurvich TPIS 1996 pt1 p139; pt2 p106.
 2 tpis96 AL  1.00H   1.00    0.00    0.00    0.00 0   27.9894780     249250.804
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8668.104
-3.759114030D+04 5.089002230D+02 1.128086896D+00 3.988660910D-03-2.150790303D-07
-2.176790819D-09 1.020805902D-12              2.644431827D+04 1.650021856D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8668.104
 6.802018430D+06-2.178416933D+04 3.032713047D+01-1.503343597D-02 4.492142360D-06
-6.178450370D-10 3.115205260D-14              1.658301221D+05-1.876766425D+02
ALHCL          Hf0 & cons: Gurvich TPIS 1996 pt1 p178; pt2 p138.
 2 tpis96 AL  1.00H   1.00CL  1.00    0.00    0.00 0   63.4421780      10521.966
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10886.572
 3.587169760D+04-5.916249990D+02 6.944542380D+00-2.511543148D-03 6.471332550D-06
-5.642277140D-09 1.715950436D-12              2.750930479D+03-9.903752973D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10886.572
-1.683915330D+05-8.862301790D+02 8.062379400D+00-9.200551470D-04 3.949817220D-07
-6.401086760D-11 3.578354100D-15              3.641504850D+03-1.800687603D+01
ALHCL2         Hf0 & cons: Gurvich TPIS 1996 pt1 p179; pt2 p140.
 2 tpis96 AL  1.00H   1.00CL  2.00    0.00    0.00 0   98.8948780    -351278.965
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13676.196
 1.184828615D+05-2.054157118D+03 1.574696513D+01-1.476257296D-02 2.065336978D-05
-1.420198850D-08 3.826279860D-12              -3.434277460D+04-5.761184971D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13676.196
 9.608063940D+04-1.485540161D+03 1.103592709D+01-3.956955200D-04 8.465843730D-08
-9.483336520D-12 4.319033530D-16              -3.669216390D+04-3.236863081D+01
ALHF           Hf0 & cons: Gurvich TPIS 1996 pt1 p164; pt2 p125.
 2 tpis96 AL  1.00H   1.00F   1.00    0.00    0.00 0   46.9878812    -182614.484
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10572.121
-9.289545100D+03 1.335515868D+02 2.772448680D+00 6.751415030D-03-4.133846140D-06
 5.865704070D-10 2.276158011D-13              -2.384685845D+04 1.228752581D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10572.121
 7.342169250D+05-3.462164130D+03 1.039714588D+01-1.750737965D-03 4.615687860D-07
-5.390414740D-11 2.340478515D-15              -2.965279722D+03-3.713172313D+01
ALHFCL         Hf0 & cons: Gurvich TPIS 1996 pt1 p184; pt2 p147.
 2 tpis96 AL  1.00H   1.00F   1.00CL  1.00    0.00 0   82.4405812    -555244.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12532.636
 1.290373237D+05-2.142099873D+03 1.485434420D+01-1.140326930D-02 1.564521768D-05
-1.067574855D-08 2.857255247D-12              -5.818303070D+04-5.483425532D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12532.636
 4.068987130D+04-1.502129854D+03 1.105214126D+01-4.031587730D-04 8.645252220D-08
-9.700659520D-12 4.423629510D-16              -6.129888110D+04-3.403564562D+01
ALHF2          Hf0 & cons: Gurvich TPIS 1996 pt1 p166; pt2 p127.
 2 tpis96 AL  1.00H   1.00F   2.00    0.00    0.00 0   65.9862844    -765299.182
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12299.975
 1.050181431D+05-1.398654202D+03 9.166334840D+00 3.867286870D-03-4.830841090D-06
 3.099287181D-09-8.440702990D-13              -8.659048800D+04-2.557299683D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12299.975
-4.419947300D+03-1.612826324D+03 1.113336052D+01-4.351812660D-04 9.344396160D-08
-1.049431425D-11 4.788333980D-16              -8.606916190D+04-3.676383785D+01
ALH2           D0 & cons: Gurvich TPIS 1996 pt1 p142; pt2 p107.
 2 tpis96 AL  1.00H   2.00    0.00    0.00    0.00 0   28.9974180     276774.934
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10090.834
 1.455182996D+04-2.153768996D+02 5.144370230D+00-3.965222030D-03 1.340900203D-05
-1.216744854D-08 3.743107130D-12              3.311037940D+04-3.608799711D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10090.834
 1.432910601D+05-2.365907684D+03 9.085667190D+00-1.308536612D-03 4.777191360D-07
-7.324721890D-11 3.997900940D-15              4.485951850D+04-3.220814285D+01
ALH2CL         Hf0 & cons: Gurvich TPIS 1996 pt1 p179; pt2 p139.
 2 tpis96 AL  1.00H   2.00CL  1.00    0.00    0.00 0   64.4501180    -106345.406
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11253.251
 9.303828980D+04-1.328188016D+03 9.424763590D+00-3.277660590D-03 1.004231609D-05
-8.948123090D-09 2.708031665D-12              -7.647437930D+03-2.682512913D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11253.251
 3.166929930D+05-3.094037914D+03 1.215872020D+01-8.248269590D-04 1.765027123D-07
-1.977372723D-11 9.006176280D-16              2.411845642D+03-4.718391553D+01
ALH2F          Hf0 & cons: Gurvich TPIS 1996 pt1 p165; pt2 p126.
 2 tpis96 AL  1.00H   2.00F   1.00    0.00    0.00 0   47.9958212    -316655.854
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10764.801
 8.906039290D+04-9.750803930D+02 5.870772320D+00 6.896663690D-03-4.045817280D-06
 7.219318660D-10 7.329846740D-14              -3.425302600D+04-9.387539141D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10764.801
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 2.711514962D+05-3.169623480D+03 1.221401118D+01-8.465600260D-04 1.812341995D-07
-2.030947985D-11 9.251825820D-16              -2.259217746D+04-4.941337333D+01
ALH3            D0 & cons: Gurvich TPIS 1996 pt1 p145; pt2 p109.
 2 tpis96 AL  1.00H   3.00    0.00    0.00    0.00 0   30.0053580     128896.080
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10410.580
 1.481207909D+04-2.836495340D+01 2.507597126D+00 7.315920510D-03 2.331766687D-06
-6.389209890D-09 2.456885069D-12              1.463189428D+04 8.313187700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10410.580
 5.885458550D+05-4.595785660D+03 1.320893344D+01-1.226849004D-03 2.626580824D-07
-2.943725869D-11 1.341177648D-15              3.991716950D+04-6.181829295D+01
ALI             D0,Props:TPIS 1996 pt1 p191 pt2 p153.
 2 tpis96 AL  1.00I   1.00    0.00    0.00    0.00 0  153.8860080      67395.017
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9751.117
 1.870854131D+03-1.543184003D+02 5.074391880D+00-1.120584830D-03 1.386302156D-06
-8.540782280D-10 2.180358492D-13              7.517443690D+03 6.688267622D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9751.117
 4.752817920D+05-1.198028588D+03 5.433685360D+00-1.004479306D-04-1.005928846D-07
 4.568173190D-11-3.960201360D-15              1.464627816D+04-3.141199746D+00
ALI2            Hf0 & cons: Gurvich TPIS 1996 pt1 p193; pt2 p154.
 2 tpis96 AL  1.00I   2.00    0.00    0.00    0.00 0  280.7904780     -33812.954
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13923.046
 1.423413595D+04-4.646575690D+02 8.722674910D+00-3.560519290D-03 4.188682290D-06
-2.616026962D-09 6.720195510D-13              -3.846133330D+03-1.073076578D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13923.046
-3.355999020D+05 4.743347940D+02 7.106501390D+00-5.529965340D-04 3.161480314D-07
-5.515489160D-11 3.174155820D-15              -9.785488850D+03-5.602275944D-01
ALI3            Hf0 & cons: Gurvich TPIS 1996 pt1 p195; pt2 p156.
 2 tpis96 AL  1.00I   3.00    0.00    0.00    0.00 0  407.6949480    -191330.433
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19003.567
 2.706032439D+04-7.559936810D+02 1.271396349D+01-5.466884090D-03 6.297618920D-06
-3.864209610D-09 9.774132440D-13              -2.220966921D+04-2.847883861D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19003.567
-6.357427470D+04-1.578772280D+01 1.001249733D+01-5.228673120D-06 1.196173520D-09
-1.409194490D-13 6.671276390D-18              -2.611455525D+04-1.247999813D+01
ALN             D0,Props:TPIS 1996 pt1 p204; pt2 p164.
 2 tpis96 AL  1.00N   1.00    0.00    0.00    0.00 0   40.9882780     438829.011
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9265.111
 2.716645079D+04-2.543491110D+02 3.538987720D+00 5.296256160D-03-9.845700610D-06
 8.452209040D-09-2.592304568D-12              5.309994910D+04 5.399436684D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9265.111
 3.821214220D+06-1.067776595D+04 1.449174222D+01-3.727227130D-03 7.922770960D-07
-8.086892210D-11 2.893539736D-15              1.205236340D+05-7.288584973D+01
ALO             D0,TabData(extrap):TPIS 1996 pt1 p122; pt2 p96.
 3 tpis96 AL  1.00O   1.00    0.00    0.00    0.00 0   42.9809380      67319.006
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8788.106
-7.683391100D+03 2.957969549D+02 4.808108440D-01 1.169224855D-02-1.595428871D-05
 1.060766814D-08-2.647888708D-12              5.843672170D+03 2.160997839D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8788.106
 1.565721161D+04 3.855741010D+03-5.926079780D+00 9.050960420D-03-2.930661549D-06
 4.238529070D-10-2.280655341D-14              -1.331694655D+04 6.830663436D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8788.106
 4.165661210D+07-3.768608760D+04 1.547867956D+01-9.568730340D-04 2.493109541D-08
 6.688940290D-14-8.998673700D-18              2.957786517D+05-9.427715804D+01
ALO+            JANAF 12/79 JPCRD v14 sup 1 1985.
 2 J12/79 AL  1.00O   1.00E  -1.00    0.00    0.00 0   42.9803894     993004.798
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 2.941443400D+00 5.259216800D-03-7.343907300D-06
 5.331678300D-09-1.578333600D-12              1.183746900D+05 9.735382485D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.190846700D+00 6.935819800D-04-3.445999900D-07
 7.617232700D-11-5.903240000D-15              1.180743900D+05 3.529519785D+00
ALO-            Estim.Data:Gurvich,TPIS,1996 pt1 p125; pt2 p98.
 2 g11/97 AL  1.00O   1.00E   1.00    0.00    0.00 0   42.9814866    -272921.782
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8744.718
 2.078075267D+04 2.859351226D+00 1.901912370D+00 7.301045660D-03-9.139769870D-06
 5.652983190D-09-1.396787103D-12              -3.359267730D+04 1.296339858D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8744.718
-6.971948290D+04-2.320553036D+02 4.672784330D+00-4.266447040D-05 1.632506336D-08
-1.727134051D-12 8.136840640D-17              -3.307718930D+04-2.155922595D+00
ALOCL           Hf0 & cons: Gurvich TPIS 1996 pt1 p176; pt2 p136.
 2 tpis96 AL  1.00O   1.00CL  1.00    0.00    0.00 0   78.4336380    -301564.570
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11906.037
-5.144627790D+03-5.886297070D+01 4.452316930D+00 9.288235090D-03-1.246894823D-05
 8.178073540D-09-2.130739934D-12              -3.759683650D+04 2.476857081D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11906.037
-1.258027706D+05-2.420565961D+02 7.681130020D+00-7.268741700D-05 1.611337534D-08
 1.852889749D-12 8.607278220D-17              -3.754326050D+04-1.475818894D+01
ALOCL2          Hf0 & cons: Gurvich TPIS 1996 pt1 p178; pt2 p137.
 2 tpis96 AL  1.00O   1.00CL  2.00    0.00    0.00 0  113.8863380    -402308.669
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15752.494
 6.902637130D+04-1.189297500D+03 1.161842739D+01 2.818279805D-04-3.145010615D-06
 3.168380650D-09-1.032375462D-12              -4.483323070D+04-3.165475922D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15752.494
-1.707713922D+05-1.180013804D+02 1.008798517D+01-3.513858040D-05 7.751187030D-09
-8.872470600D-13 4.104815440D-17              -5.124944140D+04-2.059253750D+01
ALOF            Hf0 & cons: Gurvich TPIS 1996 pt1 p163; pt2 p123.
 2 tpis96 AL  1.00O   1.00F   1.00    0.00    0.00 0   61.9793412    -572289.603
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11003.003
 7.030578360D+03-1.154575430D+02 3.378823590D+00 1.283929158D-02-1.749748388D-05
 1.162605473D-08-3.064218613D-12              -6.959381700D+04 5.994804586D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11003.003
-1.641020297D+05-3.277770290D+02 7.744519740D+00-9.788649440D-05 2.165743208D-08
-2.486541919D-12 1.153633944D-16              -6.974085090D+04-1.717253748D+01
ALOF2           Hf0 & cons: Gurvich TPIS 1996 pt1 p164; pt2 p124.
 2 tpis96 AL  1.00O   1.00F   2.00    0.00    0.00 0   80.9777444    -773649.771
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14055.387
 4.756085290D+04-6.124318360D+02 6.050223660D+00 1.559291479D-02-2.366136797D-05
 1.688366194D-08-4.690583100D-12              -9.171827490D+04-4.956258224D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14055.387
-2.496681413D+05-2.837821503D+02 1.021108125D+01-8.418303430D-05 1.855520828D-08
-2.122974022D-12 9.819319100D-17              -9.521804190D+04-2.522534812D+01
ALOF2-          JANAF 6/76 JPCRD v14 sup 1 1985.
 2 J 6/76 AL  1.00O   1.00F   2.00E   1.00    0.00 0   80.9782930   -1309625.396
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.919759700D+00 2.409401300D-02-3.608094400D-05
 2.606784800D-08-7.380837900D-12              -1.591815200D+05 1.183108219D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.614278600D+00 1.578459600D-03-7.002911500D-07
 1.372921200D-10-9.901398500D-15              -1.604033600D+05-1.587925081D+01
ALOH            Hf0 & cons: Gurvich TPIS 1996 pt1 p146; pt2 p110.
 2 tpis96 AL  1.00O   1.00H   1.00    0.00    0.00 0   43.9888780    -192762.171
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10351.931
 5.876283830D+04-9.449134210D+02 7.820445850D+00 5.862938080D-04-4.084232910D-06
 4.587629960D-09-1.564049663D-12              -1.993296951D+04-2.064957915D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10351.931
 7.882007210D+05-2.263655763D+03 7.823939000D+00 1.821250621D-04-8.263937190D-08
 1.265442255D-11-6.876114510D-16              -1.039818406D+04-2.209020907D+01
ALOH+           JANAF 12/67 JPCRD v14 sup 1 1985.
 2 J12/67 AL  1.00O   1.00H   1.00E  -1.00    0.00 0   43.9883294     543933.041
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.960343900D+00 7.919114000D-03-2.285795900D-06
-4.010378900D-09 2.570759600D-12               6.451018500D+04 1.410617757D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.150198700D+00 2.892521200D-03-1.056541400D-06
 1.794516700D-10-1.158701400D-14               6.389288800D+04 2.640138086D+00
ALOH-           JANAF 12/67 JPCRD v14 sup 1 1985.
 2 J12/67 AL  1.00O   1.00H   1.00E   1.00    0.00 0   43.9894266    -230125.630
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.913020400D+00 5.953071500D-03-3.055805400D-06
-1.259870900D-09 1.288609400D-12              -2.878182700D+04 1.062246686D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.301071800D+00 2.166850300D-03-7.398864500D-07
 1.182105500D-10-7.220884100D-15              -2.913409500D+04 3.527007516D+00
ALOHCL          Hf0 & cons: Gurvich TPIS 1996 pt1 p180; pt2 p141.
 2 tpis96 AL  1.00O   1.00H   1.00CL  1.00    0.00 0   79.4415780    -373785.740
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13918.918
 1.636360341D+04-1.915959416D+02 4.711170470D+00 1.388068475D-02-1.999018454D-05
 1.439647350D-08-4.033330450D-12              -4.568083720D+04 4.644201841D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13918.918
 7.967115510D+05-2.843470502D+03 1.095559970D+01-1.099328162D-04-1.344506283D-08
 4.415893770D-12-2.973546112D-16              -2.969861461D+04-3.296114562D+01
ALOHCL2         Hf0 & cons: REFN  Constants: table 21.14 p138.
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 2 tpis96 AL  1.00O   1.00H   1.00CL  2.00    0.00 0  114.8942780    -725145.408
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17149.806
 3.971929060D+04-7.751553840D+02 9.494050900D+00 1.074401535D-02-1.676465052D-05
 1.259706562D-08-3.613178550D-12              -8.584796980D+04-1.993482077D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17149.806
 7.385915390D+05-2.863200675D+03 1.397061990D+01-1.160295609D-04-1.208288496D-08
 4.258377470D-12-2.900073942D-16              -7.293050330D+04-4.681833172D+01
ALOHF           Hf0 & cons: Gurvich TPIS 1996 pt1 p166; pt2 p128.
 2 tpis96 AL  1.00O   1.00H   1.00F   1.00    0.00 0   62.9872812    -574211.575
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13315.081
-1.556003336D+03 2.886581999D+02 7.703793290D-01 2.450406329D-02-3.417811010D-05
 2.388932902D-08-6.570480510D-12              -7.177222560D+04 2.453071801D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13315.081
 7.557113130D+05-2.936702803D+03 1.102455104D+01-1.373078030D-04-7.432816160D-09
 3.729981220D-12-2.657027781D-16              -5.340130900D+04-3.527397302D+01
ALOHF2          Hf0 & cons: Gurvich TPIS 1996 pt1 p168; pt2 p130.
 2 tpis96 AL  1.00O   1.00H   1.00F   2.00    0.00 0   81.9856844   -1141510.711
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15428.498
 1.738263538D+04-1.307687299D+02 3.312381920D+00 2.784734099D-02-3.982363210D-05
 2.809344456D-08-7.764574200D-12              -1.384133568D+05 1.004739945D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15428.498
 6.530119920D+05-3.034017232D+03 1.409719788D+01-1.663681799D-04-1.011564183D-09
 2.993805003D-12-2.315956955D-16              -1.223052213D+05-5.151210690D+01
ALO2            D0 & cons: Gurvich,TPIS,1996,pt1,p126-8.
 2 tpis96 AL  1.00O   2.00    0.00    0.00    0.00 0   58.9803380     -38647.476
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13361.628
 4.338346490D+04-4.735104290D+02 6.001615700D+00 7.094695330D-03-1.129146941D-05
 8.252970240D-09-2.327732033D-12              -3.824985940D+03-4.829452926D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13361.628
 1.187090135D+05-8.335299180D+02 8.309268680D+00-3.538503860D-04 5.966631110D-08
 4.074618870D-14-3.516026330D-16              -2.032069600D+03-1.715040246D+01
ALO2-           D0 & cons: Gurvich,TPIS,1996,pt1,p127-9.
 2 tpis96 AL  1.00O   2.00E   1.00    0.00    0.00 0   58.9808866    -452561.855
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10644.677
 1.178722617D+05-1.507234939D+03 9.524966660D+00-5.213009120D-04-1.586266115D-06
 1.700036684D-09-5.300305660D-13              -4.825320110D+04-3.081340803D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10644.677
-1.872563912D+05-2.338468077D+02 7.676032970D+00-7.091792730D-05 1.576266909D-08
-1.815918677D-12 8.446800260D-17              -5.594541050D+04-1.773724471D+01
AL(OH)2         Hf0 & cons: Gurvich TPIS 1996 pt1 p149; pt2 p113.
 2 tpis96 AL  1.00O   2.00H   2.00    0.00    0.00 0   60.9962180    -507660.670
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14027.535
 4.397316910D+03 1.327680339D+02 1.093947024D+00 3.054059173D-02-4.375943350D-05
 3.174617430D-08-9.004259400D-12              -6.315437390D+04 2.101977655D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14027.535
 1.669643735D+06-5.924738280D+03 1.549480264D+01-5.383488080D-04 5.413044530D-08
-1.196022328D-12-1.082001733D-16              -2.697525061D+04-6.617911543D+01
AL(OH)2CL       Hf0 & cons: Gurvich TPIS 1996 pt1 p181; pt2 p142.
 2 tpis96 AL  1.00O   2.00H   2.00CL  1.00    0.00 0   96.4489180    -859056.724
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17222.037
 2.477879709D+04-4.454577210D+02 5.928470200D+00 2.730162734D-02-4.041405370D-05
 2.974210410D-08-8.477150600D-12              -1.033778030D+05-3.679945445D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17222.037
 1.603911487D+06-5.767232240D+03 1.817772266D+01-3.691816150D-04 1.137918702D-08
 4.083079400D-12-3.641323430D-16              -7.118699850D+04-7.757542241D+01
AL(OH)2F        Hf0 & cons: Gurvich TPIS 1996 pt1 p167; pt2 p129.
 2 tpis96 AL  1.00O   2.00H   2.00F   1.00    0.00 0   79.9946212   -1069628.708
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16472.051
 2.132812662D+04-1.932900224D+02 3.069174664D+00 3.555017330D-02-5.181158330D-05
 3.753520280D-08-1.059220701D-11              -1.295797992D+05 1.001897011D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16472.051
 1.559238236D+06-5.841273030D+03 1.823229919D+01-3.907805420D-04 1.610928938D-08
 3.544784060D-12-3.393453880D-16              -9.623100890D+04-7.971351802D+01
AL(OH)3         Hf0,cons: TPIS 1996 pt1 p150; pt2 p115.
 2 tpis96 AL  1.00O   3.00H   3.00    0.00    0.00 0   78.0035580   -1012667.542
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17594.767
-1.402475452D+04 3.696073460D+02-2.979600650D-01 4.929859350D-02-6.981572280D-05
 5.014801700D-08-1.412480165D-11              -1.255260760D+05 2.711490074D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17594.767
 2.477063616D+06-8.968617250D+03 2.280320998D+01-8.320292250D-04 8.663494430D-08
-2.420287082D-12-1.331746442D-16              -7.015278640D+04-1.121899198D+02
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ALS             Hf0,Props:TPIS 1996 pt1 p197; pt2 p158.
 2 tpis96 AL  1.00S   1.00    0.00    0.00    0.00 0   59.0475380     232682.009
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9088.109
 2.611742801D+04-3.470673890D+02 4.436204590D+00 3.340168210D-03-8.410199670D-06
 8.508185110D-09-2.780868507D-12                2.863779062D+04 7.522959526D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9088.109
 8.909844290D+06-2.507677454D+04 2.893456134D+01-9.839766820D-03 2.045319809D-06
-2.087970890D-10 8.152792520D-15                1.885761615D+05-1.786036203D+02
ALS2            D0,cons: TPIS 1996 pt1 p198; pt2 p159.
 2 tpis96 AL  1.00S   2.00    0.00    0.00    0.00 0   91.1135380     248535.279
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14428.779
 4.252335410D+04-7.764603300D+02 9.801068960D+00-3.910680090D-03 3.875695970D-06
-2.082025593D-09 4.682935890D-13                3.167961540D+04-2.178094603D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14428.779
-6.852563540D+04-2.671667739D+01 7.520193860D+00-8.148565100D-06 1.811865152D-09
-2.086958125D-13 9.703246380D-18                2.758362737D+04-7.873457337D+00
AL2             D0,TabData:TPIS 1996 pt1 p118; pt2 p95.
 2 tpis96 AL  2.00    0.00    0.00    0.00    0.00 0   53.9630760     501301.722
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10139.122
-5.281509650D+03-1.727374523D+01 4.604077010D+00-2.616467770D-04 6.302319970D-07
-3.290938590D-10 8.888365140D-14                5.900706390D+04 3.060188921D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10139.122
-2.320724102D+06 9.218707890D+03-9.446951870D+00 9.999920010D-03-3.154798085D-06
 4.361544810D-10-2.241157240D-14                2.904589544D+03 9.960320745D+01
AL2Br6          Hf0 & cons: Gurvich TPIS 1996 pt1 p190; pt2 p152.
 2 tpis96 AL  2.00BR  6.00    0.00    0.00    0.00 0  533.3870760    -942422.811
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38217.189
 6.483319700D+04-1.947687811D+03 2.886989822D+01-1.365825785D-02 1.557883731D-05
-9.486942000D-09 2.385519396D-12               -1.101526833D+05-1.025934782D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38217.189
-1.731829490D+05-4.342299780D+01 2.203414210D+01-1.421187503D-05 3.238631340D-09
-3.803879760D-13 1.796525455D-17               -1.202338355D+05-6.201054950D+01
AL2C2           Hf0 & cons: Gurvich TPIS 1996 pt1 p206; pt2 p167.
 2 tpis96 AL  2.00C   2.00    0.00    0.00    0.00 0   77.9844760     544978.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16165.001
 1.110987147D+04-3.502434230D+02 8.598856000D+00 1.832528671D-03 1.035743392D-06
-2.091649890D-09 7.716068700D-13                6.492764190D+04-1.645080239D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16165.001
 1.597651967D+05-1.644007203D+03 1.164643675D+01-4.379215430D-04 9.369640110D-08
-1.049615854D-11 4.780468930D-16                7.204889810D+04-3.648164252D+01
AL2CL6          Hf0 & cons: Gurvich TPIS 1996 pt1 p175; pt2 p135.
 2 tpis96 AL  2.00CL  6.00    0.00    0.00    0.00 0  266.6792760   -1296876.242
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       34147.090
 1.340935279D+05-3.001037953D+03 3.143000879D+01-1.700408496D-02 1.786540089D-05
-1.015419943D-08 2.409630451D-12               -1.471830046D+05-1.274445425D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       34147.090
-2.752975554D+05-9.248235970D+01 2.207058224D+01-2.870537915D-05 6.423325690D-09
-7.436585200D-13 3.472064670D-17               -1.629157014D+05-7.091603141D+01
AL2F6           Hf0 & cons: Gurvich TPIS 1996 pt1 p160; pt2 p122.
 2 tpis96 AL  2.00F   6.00    0.00    0.00    0.00 0  167.9534952   -2632491.231
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26064.089
 1.915061289D+05-3.168240250D+03 2.245374802D+01 1.271532036D-02-2.488697302D-05
 1.955252096D-08-5.712084890D-12               -3.049962550D+05-9.396473101D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26064.089
-5.852982610D+05-5.450571990D+02 2.240686320D+01-1.627323704D-04 3.595225040D-08
-4.121201440D-12 1.909095384D-16               -3.219683910D+05-8.589867941D+01
AL2I6           Hf0 & cons: Gurvich TPIS 1996 pt1 p196; pt2 p157.
 2 tpis96 AL  2.00I   6.00    0.00    0.00    0.00 0  815.3898960    -487747.035
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       40920.966
 2.587571514D+04-1.280719742D+03 2.677715820D+01-9.913018470D-03 1.168760413D-05
-7.303918530D-09 1.874532749D-12               -5.891105550D+04-8.330209321D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       40920.966
-1.210112399D+05-2.467542774D+01 2.201992650D+01-8.462022590D-06 1.957831901D-09
-2.326573151D-13 1.108910373D-17               -6.548523750D+04-5.528536481D+01
AL2O            D0 & cons: Gurvich TPIS 1996 pt1 p129; pt2 p101.
 2 tpis96 AL  2.00O   1.00    0.00    0.00    0.00 0   69.9624760    -148611.286
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12776.514
 7.776530700D+03-1.294235361D+02 4.912509520D+00 8.604223450D-03-1.217703648D-05
 8.314634870D-09-2.237722201D-12               -1.886512879D+04-2.806368311D-02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12776.514
-1.171074351D+05-1.783009166D+02 7.633215360D+00-5.335931770D-05 1.180702791D-08
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-1.355444579D-12 6.287323890D-17              -1.947580149D+04-1.415764167D+01
AL2O+           JANAF 12/79 JPCRD v14 sup 1 1985.
 2 J12/79 AL  2.00O   1.00E  -1.00    0.00    0.00 0   69.9619274     652444.086
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.104573600D+00 1.197835100D-02-1.852258900D-05
 1.375669100D-08-3.986742300D-12              7.685270300D+04 5.102572437D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.879785500D+00 7.074987700D-04-3.141924400D-07
 6.164098300D-11-4.447869800D-15              7.627075600D+04-8.331814463D+00
AL2O2           D0 & cons: Gurvich TPIS 1996 pt1 p131; pt2 p102.
 2 tpis96 AL  2.00O   2.00    0.00    0.00    0.00 0   85.9618760    -403095.587
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15842.613
-1.940560042D+04 2.508489836D+02 3.621403790D+00 1.951385302D-02-2.560329071D-05
 1.662721576D-08-4.312396200D-12             -5.172697280D+04 9.923995945D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15842.613
-1.940611656D+05-4.609752430D+02 1.084375637D+01-1.376042893D-04 3.044733119D-08
-3.496193920D-12 1.622305079D-16             -4.963055780D+04-2.946538090D+01
AL2O2+          JANAF 12/79 JPCRD v14 sup 1 1985.
 2 J12/79 AL  2.00O   2.00E  -1.00    0.00    0.00 0   85.9613274     567422.008
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.342190400D+00 2.811124900D-02-4.954717800D-05
 4.050975200D-08-1.261031000D-11              6.636250600D+04 9.290241635D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.275169300D+00 8.358722300D-04-3.736160800D-07
 7.360516800D-11-5.326279400D-15              6.526406800D+04-1.867725864D+01
AL2O3           D0 & cons: Gurvich TPIS 1996 pt1 p137; pt2 p105.
 2 tpis96 AL  2.00O   3.00    0.00    0.00    0.00 0  101.9612760    -546890.530
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19598.070
-7.443374320D+03 8.829004210D+01 5.264662640D+00 2.507678848D-02-3.434541650D-05
 2.302516980D-08-6.122529280D-12             -6.872685950D+04 2.202324298D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19598.070
-2.777784969D+05-4.917465930D+02 1.386703888D+01-1.469381940D-04 3.250406490D-08
-3.730867350D-12 1.730444284D-16             -6.790757850D+04-4.375559873D+01
AL2S            D0,cons: TPIS 1996 pt1 p199; pt2 p160.
 2 tpis96 AL  2.00S   1.00    0.00    0.00    0.00 0   86.0290760     220679.131
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14003.931
 4.094624370D+04-7.797172470D+02 9.814423100D+00-3.940339820D-03 3.912465430D-06
-2.105891677D-09 4.746001080D-13              2.833963305D+04-2.465065808D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14003.931
-7.043437370D+04-2.676376869D+01 7.520233820D+00-8.166123060D-06 1.816026040D-09
-2.091989298D-13 9.727537700D-18              2.422718377D+04-1.066579238D+01
AL2S2           D0,cons: TPIS 1996 pt1 p200; pt2 p161.
 2 tpis96 AL  2.00S   2.00    0.00    0.00    0.00 0  118.0950760     135287.321
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18099.521
 6.614587320D+04-1.111319537D+03 1.257007304D+01-1.456053256D-03-5.851627110D-07
 1.390055053D-09-5.496468200D-13              1.914456895D+04-3.600274552D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18099.521
-1.377806456D+05-7.705032500D+01 1.055723566D+01-2.277554487D-05 5.007682850D-09
-5.715862120D-13 2.637999240D-17              1.313336091D+04-2.256849054D+01
Ar              Ref-Elm. Spec: NSRDS-NBS 35 1971.
 3 g 3/98 AR  1.00    0.00    0.00    0.00    0.00 0   39.9480000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02 4.379674910D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.010538475D+01-5.992661070D-02 2.500069401D+00-3.992141160D-08 1.205272140D-11
-1.819015576D-15 1.078576636D-19             -7.449939610D+02 4.379180110D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-9.951265080D+08 6.458887260D+05-1.675894697D+02 2.319933363D-02-1.721080911D-06
 6.531938460D-11-9.740147729D-16             -5.078300340D+06 1.465298484D+03
Ar+             Levels: NSRDS-NBS 35 1971; IP:NSRDS-NBS 34 1970.
 3 g 3/97 AR  1.00E  -1.00    0.00    0.00    0.00 0   39.9474514    1526778.407
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.988
-5.731209170D+04 7.930791470D+02-1.717121217D+00 1.044184018D-02-1.180207501D-05
 6.528134780D-09-1.447558130D-12              1.790572230D+05 2.949150950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.988
-3.835965400D+05 8.162019700D+02 2.301342628D+00-4.952983770D-06 1.205108477D-08
-2.185050286D-12 1.265493898D-16              1.771811455D+05 7.947507480D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.988
 1.017372837D+07-6.685104100D+03 4.460953790D+00-3.034165287D-04 2.623479563D-08
-1.205115834D-12 2.303806883D-17              2.354353541D+05-1.044519298D+01
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B               JPCA v102 n18 1998 p2995. Spec:JPCRD v8 n1 1979 p63.
 3 g 9/98 B   1.00    0.00    0.00    0.00    0.00 0   10.8110000     575598.760
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6316.060
 1.182394638D+02-7.009916910D-02 2.500236159D+00-4.584213700D-07 5.123185830D-10
-3.057217674D-13 7.533815325D-17                6.848359080D+04 4.209501920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6316.060
-1.072659610D+05 3.225307160D+02 2.126407232D+00 2.106579339D-04-5.937129160D-08
 7.377427990D-12-2.282443381D-16                6.643413100D+04 6.877069670D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6316.060
-4.150001310D+08 2.329576796D+05-4.720913710D+01 4.877655960D-03-2.069413791D-07
 3.233519090D-12-1.824076527D-18               -1.802904743D+06 4.439617640D+02
B+              Spec: NSRDS-NBS 35 1971. IP:NSRDS-NBS 34 1970.
 3 g 1/98 B   1.00E  -1.00    0.00    0.00    0.00 0   10.8104514    1371716.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 7.849791190D-02-8.947480950D-04 2.500004085D+00-9.577271230D-09 1.218136411D-11
-7.986752520D-15 2.113769829D-18                1.642332906D+05 2.419053631D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-8.911548030D+03 4.587790090D+00 2.531500086D+00-4.903949100D-05 2.853326582D-08
-7.382175910D-12 7.120721560D-16                1.641778950D+05 2.238669780D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-7.977322890D+08 4.734044940D+05-1.055286044D+02 1.170310076D-02-6.075531110D-07
 1.484174716D-11-1.328323987D-16               -3.610391700D+06 9.497399750D+02
B-              JPCRD v14 n3 1985 p731.
 3 g 1/98 B   1.00E   1.00    0.00    0.00    0.00 0   10.8115486     532032.698
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6272.598
 2.201568105D+01-4.740468880D-03 2.500014238D+00-2.497056599D-08 2.556360708D-11
-1.415274780D-14 3.271770710D-18                6.324318340D+04 4.616367290D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6272.598
 2.118018248D+01 2.070697496D-04 2.499999729D+00 1.456693631D-10-3.888571760D-14
 5.090598630D-18-2.601566168D-22                6.324315600D+04 4.616455830D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6272.598
-1.311386485D+02 9.028908800D-02 2.499978572D+00 2.606391052D-09-1.716068068D-13
 5.810865540D-18-7.925029090D-23                6.324243870D+04 4.616640300D+00
BBr             Cons & D0: TPIS 1996 pt1 p91 pt2 p70.
 2 g 9/98 B   1.00BR  1.00    0.00    0.00    0.00 0   90.7150000     240952.358
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8997.058
 3.796093500D+04-4.976096020D+02 5.267008200D+00-3.742840190D-05-1.131544370D-06
 1.261945702D-09-4.288811880D-13                3.038125367D+04-4.353407330D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8997.058
 2.536858027D+05-6.405909500D+02 4.666823470D+00 4.175486390D-04-2.963714868D-07
 7.519119540D-11-4.835368320D-15                3.189084340D+04-8.255870910D-01
BBr2            Cons & D0: TPIS 1996 pt1 p92 pt2 p71.
 2 g 9/98 B   1.00BR  2.00    0.00    0.00    0.00 0  170.6190000      97828.617
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12200.717
 6.516550710D+04-9.029590760D+02 8.063817800D+00 1.129849010D-03-4.195482390D-06
 3.965658770D-09-1.283029835D-12                1.470466408D+04-1.336453164D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12200.717
-4.191633370D+05 4.157688470D+02 7.148169830D+00-5.689590750D-04 3.195441770D-07
-5.553176990D-11 3.191136760D-15                6.118982050D+03-5.502759620D+00
BBr3            Cons & Hf: TPIS 1996 pt1 p93 pt2 p72.
 2 tpis96 B   1.00BR  3.00    0.00    0.00    0.00 0  250.5230000    -205300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15702.797
 3.968073690D+04-6.331087160D+02 8.054551570D+00 9.777571300D-03-1.614866025D-05
 1.216119883D-08-3.516539610D-12               -2.366723308D+04-1.106099390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15702.797
-1.901046795D+05-1.503627687D+02 1.010999896D+01-4.323095110D-05 9.409696190D-09
-1.065218470D-12 4.883048770D-17               -2.742553062D+04-1.997496003D+01
BC              Props & D0: TPIS 1996 pt1 p108 pt2 p86.
 2 g 9/98 B   1.00C   1.00    0.00    0.00    0.00 0   22.8217000     838161.905
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8735.105
-3.915758000D+04 7.284538060D+02-1.552743361D+00 1.552898673D-02-1.976857863D-05
 1.272066405D-08-3.229982780D-12                9.644913680D+04 3.248204466D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8735.105
-2.346280674D+06 6.450751300D+03-2.619532384D+00 3.339160500D-03-4.508022140D-07
 1.351919576D-11 8.265104270D-16                5.786685070D+04 5.037884876D+01
BC2             Cons & D0:TPIS 1996 pt1 p109, pt2 p87.
 2 g 9/98 B   1.00C   2.00    0.00    0.00    0.00 0   34.8324000     801258.725
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11687.825
-2.987422175D+04 3.643126580D+02 2.963469415D+00 6.561750150D-03-3.539767240D-06
 1.927356029D-10 3.118724866D-13                9.304835730D+04 1.083424193D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11687.825
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 1.525485889D+06-5.987862380D+03 1.408384855D+01-3.747499800D-03 1.081927223D-06
-1.378744645D-10 6.473822000D-15              1.311204013D+05-6.337215498D+01
BCL            Cons & D0: TPIS 1996 pt1 p73 pt2 p51.
 2 g 9/98 B   1.00CL  1.00    0.00    0.00    0.00 0   46.2637000    183173.437
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8861.337
 2.202458989D+04-1.700511155D+02 3.066075869D+00 5.595070180D-03-8.460870410D-06
 6.084733410D-09-1.702889433D-12              2.197402537D+04 6.388969190D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8861.337
-7.421262540D+04 2.638090127D+02 3.600227650D+00 1.018866266D-03-4.666184120D-07
 9.849002030D-11-6.468818170D-15              1.912726480D+04 5.235308150D+00
BCL+           JANAF 6/68 JPCRD v14 sup 1 1985.
 2 J 6/68 B   1.00CL  1.00E  -1.00    0.00    0.00 0   46.2631514   1234312.340
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.812419700D+00 4.600639200D-03-4.811996200D-06
 1.967221600D-09-1.383780200D-13              1.474484900D+05 9.156682450D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.106088800D+00 4.727417000D-04-1.792858400D-07
 3.241613700D-11-2.054575800D-15              1.471309700D+05 2.642729450D+00
BCLOH          Cons & D0: TPIS 1996 pt1 p83 pt2 p61.
 2 g 9/98 B   1.00CL  1.00O   1.00H   1.00    0.00 0   63.2710400   -234005.381
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12431.519
-2.898427288D+04 6.894046580D+02-2.288138069D+00 3.349428620D-02-4.725225980D-05
 3.326981310D-08-9.224238860D-12             -3.261981100D+04 3.976885940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12431.519
 7.027738440D+05-2.857391274D+03 1.091175840D+01-8.107709340D-05-2.124440337D-08
 5.409912440D-12-3.464153840D-16             -1.307221888D+04-3.585169510D+01
BCL(OH)2       Cons & Hf0: TPIS 1996 pt1 p85 pt2 p62.
 2 tpis96 B   1.00CL  1.00O   2.00H   2.00    0.00 0   80.2783800   -805387.658
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13565.103
 8.072623010D+04-8.594619820D+02 2.705039614D+00 3.878799620D-02-5.721734350D-05
 4.145850330D-08-1.168536754D-11             -9.379910740D+04 7.134977090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13565.103
 1.423878191D+06-5.849704070D+03 1.792165219D+01-2.009909087D-04-3.393435780D-08
 9.838560760D-12-6.472678820D-16             -6.474261760D+04-8.100400080D+01
BCL2           Cons & Hf0: TPIS 1996 pt1 p74 pt2 p52.
 2 tpis96 B   1.00CL  2.00    0.00    0.00    0.00 0   81.7164000    -60881.490
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11513.621
 3.598879420D+04-3.602826500D+02 4.157685450D+00 1.152877450D-02-1.816567395D-05
 1.341714418D-08-3.840822860D-12             -6.765107050D+03 5.182300860D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11513.621
 3.501403130D+05-1.662203590D+03 8.839534720D+00-9.772544110D-04 2.467356248D-07
-2.501151018D-11 8.722954560D-16              5.682909440D+02-2.148349445D+01
BCL2+          JANAF 12/70 JPCRD v14 sup 1 1985.
 2 J12/70 B   1.00CL  2.00E  -1.00    0.00    0.00 0   81.7158514    674064.428
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.270493100D+00 1.060379100D-02-1.422983800D-05
 8.537283100D-09-1.834967100D-12              7.943601600D+04 4.076450690D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.926662700D+00 6.777763300D-04-3.210149600D-07
 6.834442200D-11-5.007359200D-15              7.885782200D+04-8.934626610D+00
BCL2-          JANAF 6/72 JPCRD v14 sup 1 1985.
 2 J 6/72 B   1.00CL  2.00E   1.00    0.00    0.00 0   81.7169486   -146439.370
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.235879100D+00 1.169021900D-02-1.477825900D-05
 8.218154600D-09-1.565791300D-12             -1.898181500D+04 1.069001040D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.351821800D+00 7.702884800D-04-4.469986300D-07
 1.383117800D-10-1.322199500D-14             -1.970543200D+04-4.774720730D+00
BCL2OH         Cons & Hf0: TPIS 1996 pt1 p86 pt2 p63.
 2 tpis96 B   1.00CL  2.00O   1.00H   1.00    0.00 0   98.7237400   -604917.444
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14051.769
 2.099755170D+04-2.470699169D+02 2.578761742D+00 3.120362393D-02-4.545314050D-05
 3.242011770D-08-9.039822660D-12             -7.309028620D+04 1.273657699D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14051.769
 5.878113790D+05-2.982969317D+03 1.400662004D+01-1.194189832D-04-1.269775742D-08
 4.422892190D-12-3.004089365D-16             -5.824168070D+04-5.150859140D+01
BCL3           Cons & Hf: TPIS 1996 pt1 p76 pt2 p53.
 2 tpis96 B   1.00CL  3.00    0.00    0.00    0.00 0  117.1691000   -404500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13970.666
 2.392970339D+04-4.140378860D+02 5.488035260D+00 1.648395682D-02-2.456196216D-05
 1.743876340D-08-4.845222140D-12             -4.839469840D+04-1.675366720D+00
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13970.666
-2.417408819D+05-2.921539509D+02 1.021668480D+01-8.623637100D-05 1.897792088D-08
-2.168726841D-12 1.002154013D-16              -5.074834440D+04-2.546863529D+01
BF              Cons & Hf0: TPIS 1996 pt1 p56 pt2 p36.
 2 g10/97 B   1.00F   1.00    0.00    0.00    0.00 0   29.8094032    -106931.884
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8694.670
-5.238954730D+04 8.118476640D+02-1.141614903D+00 1.161249417D-02-1.175212617D-05
 6.019232780D-09-1.238293129D-12              -1.774541998D+04 3.005086287D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8694.670
-3.746389780D+05 5.604493910D+02 3.609186110D+00 6.187216930D-04-1.778938770D-07
 2.426601527D-11-9.394651580D-16              -1.819179292D+04 3.716609290D+00
BFCL            Cons & Hf0: TPIS 1996 pt1 p86 pt2 p64.
 2 tpis96 B   1.00F   1.00CL  1.00    0.00    0.00 0   65.2621032    -279184.068
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11033.040
-2.363512735D+04 4.383168980D+02 3.918095720D-01 1.719990692D-02-2.139592424D-05
 1.337389186D-08-3.371164690D-12              -3.687166590D+04 2.668102062D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11033.040
-1.086309561D+05-5.233438480D+02 7.297504740D+00-3.054410701D-05-3.154598306D-08
 1.052290533D-11-7.615432260D-16              -3.305891210D+04-1.186587285D+01
BFCL2           Cons & Hf: TPIS 1996 pt1 p88 pt2 p66.
 2 tpis96 B   1.00F   1.00CL  2.00    0.00    0.00 0  100.7148032    -643000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.913
 4.402551240D+03-1.571398929D+02 4.016322310D+00 1.743396078D-02-2.252789060D-05
 1.433673443D-08-3.648755580D-12              -7.822452620D+04 6.886085810D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.913
-2.233613309D+05-6.440602960D+02 1.047861848D+01-1.911892367D-04 4.224887790D-08
-4.847266920D-12 2.247974725D-16              -7.740626480D+04-2.814631458D+01
BFOH            Cons & D0: TPIS 1996 pt1 p71 pt2 p48.
 2 g 9/98 B   1.00F   1.00O   1.00H   1.00    0.00 0   46.8167432    -451631.678
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11973.122
-7.563953670D+04 1.354838128D+03-5.648210110D+00 3.870274660D-02-5.037659180D-05
 3.339592640D-08-8.847822950D-12              -6.194446110D+04 5.800362820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11973.122
 7.251318090D+05-3.215620850D+03 1.117909777D+01-1.883881929D-04 2.579708080D-09
 2.665158100D-12-2.186647438D-16              -3.716808080D+04-3.978463490D+01
BF(OH)2         Cons & Hf0: TPIS 1996 pt1 p71 pt2 p49.
 2 tpis96 B   1.00F   1.00O   2.00H   2.00    0.00 0   63.8240832   -1049889.539
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12885.220
 1.381800676D+04 2.529637004D+02-3.844552040D+00 5.255140850D-02-7.193117730D-05
 4.948309910D-08-1.345922496D-11              -1.283123258D+05 4.293659370D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12885.220
 1.422037640D+06-6.257297570D+03 1.822460686D+01-3.221396450D-04-7.126739900D-09
 6.758699770D-12-5.042554540D-16              -9.186254190D+04-8.527895050D+01
BF2             Cons & Hf0: TPIS 1996 pt1 p58 pt2 p37.
 2 tpis96 B   1.00F   2.00    0.00    0.00    0.00 0   48.8078064    -499426.904
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10612.202
-6.787651760D+04 1.085903536D+03-3.023320961D+00 2.326503687D-02-2.641444147D-05
 1.515620683D-08-3.518559180D-12              -6.640918250D+04 4.431968310D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10612.202
-1.153091296D+05-8.109800120D+02 7.602709230D+00-2.409209242D-04 5.328471860D-08
-6.118797940D-12 2.839984178D-16              -5.796222170D+04-1.655644047D+01
BF2+            JANAF 12/70 JPCRD v14 sup 1 1985.
 2 J12/70 B   1.00F   2.00E  -1.00    0.00    0.00 0   48.8072578     322597.382
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 3.314647400D+00 8.644365400D-03-6.752539600D-06
 1.338366500D-09 4.511491000D-13               3.748364900D+04 5.904689780D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 5.812763800D+00 1.819342400D-03-7.710345700D-07
 1.448978200D-10-9.980915600D-15               3.679480100D+04-7.004311920D+00
BF2-            Cons & Hf0: TPIS 1996 pt1 p60 pt2 p38.
 2 tpis96 B   1.00F   2.00E   1.00    0.00    0.00 0   48.8083550    -733802.963
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10433.571
 2.109765318D+04 1.439564600D+02 2.604646296D-01 1.817373751D-02-2.241565287D-05
 1.369712886D-08-3.355952680D-12              -8.971801780D+04 2.351692604D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10433.571
-1.709920627D+05-6.156219790D+02 7.458871370D+00-1.836703248D-04 4.064363960D-08
-4.667700950D-12 2.166264840D-16              -8.741404530D+04-1.620604664D+01
BF2CL           Cons & Hf: TPIS 1996 pt1 p87 pt2 p65.
 2 tpis96 B   1.00F   2.00CL  1.00    0.00    0.00 0   84.2605064    -888000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12323.693
 4.500101250D+03-1.196284966D+02 3.198635140D+00 1.743426933D-02-1.994070287D-05
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 1.125136430D-08-2.544020371D-12              -1.076779851D+05 1.008194481D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12323.693
-2.066817398D+05-1.024447292D+03 1.075843981D+01-3.023235319D-04 6.672521470D-08
-7.649941900D-12 3.546224500D-16              -1.046936725D+05-3.229995570D+01
BF2OH           Cons & Hf0: TPIS 1996 pt1 p72 pt2 p50.
 2 tpis96 B   1.00F   2.00O   1.00H   1.00    0.00 0   65.8151464   -1092217.322
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12395.887
-7.522521650D+03 4.367121690D+02-3.128973474D+00 4.323957680D-02-5.785494040D-05
 3.885858130D-08-1.038574523D-11              -1.344259458D+05 4.139170550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12395.887
 5.760759250D+05-3.611900190D+03 1.446897640D+01-3.028293733D-04 2.764337508D-08
-1.905493170D-13-8.694971940D-17              -1.133589041D+05-5.896981510D+01
BF3             Cons & Hf: TPIS 1996 pt1 p62 pt2 p39.
 2 tpis96 B   1.00F   3.00    0.00    0.00    0.00 0   67.8062096   -1136000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11651.226
 3.465584000D+03 2.133198651D+01 1.641245191D+00 1.993755064D-02-2.150119930D-05
 1.145669081D-08-2.442285789D-12              -1.379455591D+05 1.625533544D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11651.226
-1.819767014D+05-1.405347931D+03 1.103412258D+01-4.104591050D-04 9.031277570D-08
-1.033057360D-11 4.780551830D-16              -1.323136863D+05-3.738386080D+01
BF4-            Cons & Hf0: TPIS 1996 pt1 p63 pt2 p40.
 2 tpis96 B   1.00F   4.00E   1.00    0.00    0.00 0   86.8051614   -1761265.998
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13795.643
 2.068485200D+05-2.463190805D+03 1.206414196D+01 1.102766923D-02-1.751720760D-05
 1.201346256D-08-3.150588626D-12              -2.010569206D+05-4.610826940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13795.643
-4.373241710D+05-7.759289410D+02 1.358222575D+01-2.341024178D-04 5.196915940D-08
-5.982245780D-12 2.781163206D-16              -2.127251877D+05-4.953369700D+01
BH              Props & D0: TPIS 1996 pt1 p28 pt2 p19.
 3 g 9/98 B   1.00H   1.00    0.00    0.00    0.00 0   11.8189400    456723.204
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8639.104
 2.063082550D+04-3.682502520D+02 6.071337870D+00-8.728321070D-03 1.458566459D-05
-1.036840401D-08 2.779462579D-12               5.556629140D+04-1.300392582D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8639.104
-1.098531663D+06-1.745890126D+02 8.442426810D+00-5.440196670D-03 2.718307052D-06
-4.839812210D-10 2.868523222D-14               5.112904900D+04-2.971030686D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8639.104
 1.671568144D+07-4.739239340D+04 3.002619492D+01-4.066741700D-03 2.728858457D-07
-8.930751160D-12 1.162189261D-16               3.772297760D+05-2.142712519D+02
BHCL            Cons & D0: TPIS 1996 pt1 p81 pt2 p58.
 2 g 9/98 B   1.00H   1.00CL  1.00    0.00    0.00 0   47.2716400    141418.307
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10304.807
 4.763274910D+04-4.420016520D+02 3.975645880D+00 8.541698760D-03-1.377785182D-05
 1.131521587D-08-3.569659180D-12               1.822278428D+04 3.028442880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10304.807
 3.499991720D+05-2.238404757D+03 8.711106050D+00-1.088882906D-03 4.189301090D-07
-6.568711260D-11 3.620067600D-15               2.841240364D+04-2.589567177D+01
BHCL2           Cons & Hf0: TPIS 1996 pt1 p82 pt2 p60.
 2 tpis96 B   1.00H   1.00CL  2.00    0.00    0.00 0   82.7243400    -251883.529
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11745.632
 4.419914810D+04-2.384739577D+02 1.356682235D+00 2.517866897D-02-3.632910400D-05
 2.644335581D-08-7.625044110D-12              -3.003877914D+04 1.787023528D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11745.632
 4.110996060D+05-2.858027441D+03 1.179547506D+01-6.322817970D-04 1.269551549D-07
-1.352862344D-11 5.921653510D-16              -1.617288760D+04-4.217902060D+01
BHF             Cons & D0: TPIS 1996 pt1 p68 pt2 p45.
 2 g 9/98 B   1.00H   1.00F   1.00    0.00    0.00 0   30.8173432    -76012.343
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10042.057
-4.908362260D+04 9.610760210D+02-2.919850316D+00 2.149156633D-02-2.595677863D-05
 1.693492714D-08-4.553648840D-12              -1.466925195D+04 4.160709310D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10042.057
 1.184821300D+06-4.677435180D+03 1.067328148D+01-1.606366598D-03 3.704534700D-07
-3.797882750D-11 1.432441145D-15               1.802640937D+04-4.285931170D+01
BHFCL           Cons & Hf0: TPIS 1996 pt1 p90 pt2 p69.
 2 tpis96 B   1.00H   1.00F   1.00CL  1.00    0.00 0   66.2700432    -483036.620
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11414.539
 5.761169720D+02 3.042156250D+02-9.808900360D-01 2.803843648D-02-3.676734020D-05
 2.499824138D-08-6.873421640D-12              -6.050207390D+04 3.132841413D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11414.539
 4.390778920D+05-3.137181709D+03 1.200286161D+01-7.153669340D-04 1.453878608D-07
-1.565197070D-11 6.910075060D-16              -4.232368340D+04-4.466543560D+01
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BHF2            Cons & Hf0: TPIS 1996 pt1 p69 pt2 p47.
 2 tpis96 B   1.00H   1.00F   2.00    0.00    0.00 0   49.8157464    -739613.811
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10659.347
-8.353540280D+04 1.616659766D+03-8.161405670D+00 4.153786790D-02-4.921063280D-05
 3.054165306D-08-7.786813980D-12              -9.748065460D+04 7.038630750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10659.347
 4.660876960D+05-3.728100490D+03 1.244152658D+01-8.906843190D-04 1.841732568D-07
-2.010774349D-11 8.979196590D-16              -6.978142930D+04-5.103218040D+01
BH2             Cons & D0: TPIS 1996 pt1 p32 pt2 p20.
 2 tpis96 B   1.00H   2.00    0.00    0.00    0.00 0   12.8268800     318289.275
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10002.575
 3.752797730D+04-4.877333130D+02 6.340172780D+00-6.136701630D-03 1.190254981D-05
-7.118656880D-09 1.308345772D-12              3.947668650D+04-1.290841520D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10002.575
 1.565810423D+06-6.858184340D+03 1.329759641D+01-2.705961116D-03 6.139550450D-07
-7.100581650D-11 3.293880160D-15              7.859965430D+04-6.638430200D+01
BH2CL           Cons & Hf0: TPIS 1996 pt1 p82 pt2 p59.
 2 tpis96 B   1.00H   2.00CL  1.00    0.00    0.00 0   48.2795800     -80845.754
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10426.902
 1.646638117D+04 1.277320942D+02 1.300268921D-01 1.938143193D-02-2.316389616D-05
 1.607896164D-08-4.668337650D-12              -1.112112215D+04 2.308499180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10426.902
 1.427215437D+06-6.265564340D+03 1.382183005D+01-1.313843556D-03 2.587131606D-07
-2.713845270D-11 1.172827257D-15              2.639387516D+04-6.399726240D+01
BH2F            Cons & Hf0: TPIS 1996 pt1 p69 pt2 p46.
 2 tpis96 B   1.00H   2.00F   1.00    0.00    0.00 0   31.8252832    -323956.732
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10137.922
-8.837920440D+04 1.705285929D+03-8.061246130D+00 3.643188680D-02-4.152482550D-05
 2.620135756D-08-6.930886410D-12              -4.787273410D+04 6.862087670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10137.922
 1.435082111D+06-6.625320170D+03 1.409165008D+01-1.422469060D-03 2.828724718D-07
-2.992498948D-11 1.302618926D-15              -7.937192670D+02-6.801356400D+01
BH3             Cons & Hf: TPIS 1996 pt1 p34 pt2 p21.
 2 tpis96 B   1.00H   3.00    0.00    0.00    0.00 0   13.8348200      88000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9992.015
-4.430791200D+04 6.792257290D+02 4.698919650D-01 5.702213220D-03 4.143647470D-06
-5.580210950D-09 1.680924233D-12              6.145424830D+03 2.008713776D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9992.015
 2.431957621D+06-9.585547590D+03 1.587143758D+01-2.026744757D-03 4.006226470D-07
-4.216972380D-11 1.827996789D-15              6.819014970D+04-8.715538010D+01
BH3NH3          Cons & Hf: TPIS 1996 pt1 p106 pt2 p84.
 2 tpis96 B   1.00H   6.00N   1.00    0.00    0.00 0   30.8653800    -115000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12681.530
-1.811063598D+05 3.010341543D+03-1.524271135D+01 6.215637750D-02-5.959881850D-05
 3.267429360D-08-7.751243090D-12              -2.934278877D+04 1.087399627D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12681.530
 4.354925960D+06-1.824235232D+04 3.162999830D+01-3.208243610D-03 5.885075450D-07
-5.808535530D-11 2.382578600D-15              9.438118030D+04-1.897865780D+02
BI              Cons & D0: TPIS 1996 pt1 p94 pt2 p73.
 2 g 9/98 B   1.00I   1.00    0.00    0.00    0.00 0  137.7154700     325987.502
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9142.202
 3.517449530D+04-5.445819300D+02 6.027511010D+00-2.387237926D-03 2.244796277D-06
-1.110001347D-09 2.280204403D-13              4.071910130D+04-7.288049840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9142.202
 2.132872626D+06-6.283684960D+03 1.123964343D+01-3.258856750D-03 7.064282150D-07
-4.230068930D-11-4.208078470D-16              7.797634810D+04-4.664042610D+01
BI2             Cons & D0: TPIS 1996 pt1 p95 pt2 p74.
 2 g 9/98 B   1.00I   2.00    0.00    0.00    0.00 0  264.6199400     238096.324
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12688.424
 6.640975900D+04-1.044411994D+03 9.734197240D+00-3.952557540D-03 3.165567780D-06
-1.273764644D-09 1.879968132D-13              3.205750890D+04-2.012407058D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12688.424
-3.924022230D+05 4.422902350D+02 7.129623580D+00-5.619634060D-04 3.180760520D-07
-5.537079720D-11 3.183959700D-15              2.291972638D+04-3.201793240D+00
BI3             Cons & Hf: TPIS 1996 pt1 p96 pt2 p75.
 2 tpis96 B   1.00I   3.00    0.00    0.00    0.00 0  391.5244100      21400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16933.072
 6.243114890D+04-1.002408628D+03 1.106650075D+01 1.609588058D-03-5.147250250D-06
 4.732514020D-09-1.512999796D-12              5.160348150D+03-2.420687643D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16933.072
-1.506176506D+05-8.167210610D+01 1.005937867D+01-2.319396215D-05 5.019966730D-09
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-5.654349630D-13 2.580651348D-17              -4.261687910D+02-1.617962779D+01
BN            Props & D0: TPIS 1996 pt1 p104, pt2 p83.
 2 g 9/98 B   1.00N   1.00    0.00    0.00    0.00 0   24.8177400     574726.408
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8961.108
-4.569707580D+04 6.704286070D+02 3.615089080D-02 7.339487510D-03-4.969033490D-06
 1.229031380D-09 6.340281520D-14              6.485465080D+04 2.539870138D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8961.108
-2.276932705D+05-1.025649298D+02 4.414586810D+00 2.561670989D-04-1.612994942D-08
-6.526052930D-13 5.749466120D-17              6.784465130D+04-6.778544480D-01
BO            Props & D0: TPIS 1996 pt1 p10, pt2 p8.
 3 g 9/98 B   1.00O   1.00    0.00    0.00    0.00 0   26.8104000      20406.404
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8674.104
-1.166216822D+04 9.217579390D+01 3.655498490D+00-3.118542920D-03 9.008329830D-06
-8.017789990D-09 2.472952292D-12              8.738284780D+02 4.482847390D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8674.104
 1.788600589D+04-6.309019630D+02 4.574528400D+00 1.988001643D-04-9.702963480D-08
 1.870854291D-11-1.030218131D-15              4.841311090D+03-3.398890580D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8674.104
-1.592699514D+08 1.210955629D+05-3.136823502D+01 5.110037760D-03-3.461020740D-07
 1.148046833D-11-1.504899225D-16              -9.345065760D+05 3.026123907D+02
BO-           Cons & EA: TPIS 1996 pt1 p13, pt2 p10.
 2 g 9/98 B   1.00O   1.00E   1.00    0.00    0.00 0   26.8109486    -277791.076
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8674.024
-8.242023210D+04 9.203636900D+02-2.302659981D-01 6.229904120D-03-3.157624391D-06
 1.184578107D-10 2.819228693D-13              -3.911141220D+04 2.599226838D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8674.024
 2.122804369D+05-1.262124688D+03 5.383167310D+00-3.181049100D-04 7.288988250D-08
-8.141708920D-12 3.715364390D-16              -2.706892261D+04-9.773753670D+00
BOCL          Boron oxide-chloride.Cons&Hf0:TPIS1996 pt1 p79, pt2 p55.
 2 tpis96 B   1.00O   1.00CL  1.00    0.00    0.00 0   62.2631000    -318536.695
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10607.913
 7.052380640D+04-1.315301429D+03 1.130087727D+01-1.207112050D-02 1.880516131D-05
-1.373823975D-08 3.854890160D-12              -3.355399100D+04-3.698463240D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10607.913
 1.557148487D+05-1.446254968D+03 8.509448050D+00-3.859007380D-04 8.262268820D-08
-9.261027460D-12 4.219998010D-16              -3.203589040D+04-2.372714015D+01
BOCL2         Cons & Hf0: TPIS 1996 pt1 p79 pt2 p56.
 2 tpis96 B   1.00O   1.00CL  2.00    0.00    0.00 0   97.7158000    -361565.512
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13169.650
 7.322667360D+03-2.027726965D+02 4.161924090D+00 1.733309456D-02-2.263908718D-05
 1.452275190D-08-3.719593120D-12              -4.414441880D+04 6.520414900D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13169.650
-2.297527041D+05-6.194567930D+02 1.046075518D+01-1.841620739D-04 4.071215430D-08
-4.672246550D-12 2.167237536D-16              -4.371538420D+04-2.743571136D+01
BOF           Boron oxide-fluoride.Cons&Hf0:TPIS1996 pt1 p65, pt2 p42.
 2 tpis96 B   1.00O   1.00F   1.00    0.00    0.00 0   45.8088032    -592978.311
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9988.295
 7.226802650D+04-1.131386630D+03 8.816054520D+00-4.627694570D-03 7.801299580D-06
-5.681205840D-09 1.534732094D-12              -6.711116010D+04-2.547957229D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9988.295
 1.937020297D+05-1.739112297D+03 8.695650860D+00-4.518895570D-04 9.591019080D-08
-1.067806769D-11 4.840007660D-16              -6.330152390D+04-2.702458617D+01
BOF2          Cons & Hf0: TPIS 1996 pt1 p66 pt2 p43.
 2 tpis96 B   1.00O   1.00F   2.00    0.00    0.00 0   64.8072064    -832767.700
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11611.458
 7.227794130D+03 2.148783624D+01 1.157840301D+00 2.250585296D-02-2.610731536D-05
 1.508824929D-08-3.518364850D-12              -1.013995733D+05 2.010127136D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11611.458
-2.205028861D+05-1.254238690D+03 1.092551380D+01-3.680144000D-04 8.107164940D-08
-9.281275060D-12 4.297549300D-16              -9.680447580D+04-3.482853330D+01
BOH           Boron hydroxide. Cons & Hf0:TPIS 1996 pt1 p41, pt2 p24.
 2 tpis96 B   1.00O   1.00H   1.00    0.00    0.00 0   27.8183400      -6756.578
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10031.524
-7.521410270D+04 1.391444703D+03-5.630330180D+00 2.966358811D-02-3.830835180D-05
 2.550606424D-08-6.795857210D-12              -8.341300280D+03 5.517690040D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10031.524
 8.447498570D+05-3.016982887D+03 8.083864700D+00-1.609855388D-04-2.191830959D-09
 3.127133119D-12-2.376665451D-16               1.647698495D+04-2.603227947D+01
BO2           Cons & Hf0: TPIS 1996 pt1 p14 pt2 p11.
 2 g10/97 B   1.00O   2.00    0.00    0.00    0.00 0   42.8098000    -309121.947
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10772.157
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-4.141090640D+04 7.198854610D+02-1.477629435D+00 2.277415194D-02-2.786326934D-05
 1.718462069D-08-4.278991440D-12              -4.177657690D+04 3.258458010D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10772.157
-3.834452340D+04-9.563261140D+02 8.200962780D+00-2.062130802D-04 9.872288990D-09
 8.158366760D-12-7.527519660D-16              -3.423564020D+04-2.224772278D+01
BO2-            Cons & Hf0: TPIS 1996 pt1 p16 pt2 p13.
 2 tpis96 B   1.00O   2.00E   1.00    0.00    0.00 0   42.8103486    -714493.991
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9597.541
 5.324279690D+04-7.326313030D+02 5.902470000D+00 2.437465200D-03-4.878803950D-07
-8.475724760D-10 4.080781180D-13              -8.344293680D+04-1.053931911D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9597.541
 1.199226372D+05-1.715766982D+03 8.701038220D+00-4.601242120D-04 9.867011870D-08
-1.107288516D-11 5.050183240D-16              -7.825789690D+04-2.839356505D+01
B(OH)2          Cons & D0: TPIS 1996 pt1 p46 pt2 p28.
 2 g 9/98 B   1.00O   2.00H   2.00    0.00    0.00 0   44.8256800    -425243.642
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11971.658
 1.491659222D+03 3.648184840D+02-2.906006389D+00 4.136834460D-02-5.782584220D-05
 4.069783560D-08-1.126499791D-11              -5.375483660D+04 3.888535180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11971.658
 1.557023406D+06-5.784710760D+03 1.487391235D+01-1.821804765D-04-3.803541640D-08
 1.030332746D-11-6.685889830D-16              -1.806810301D+04-6.590268900D+01
BS              Props & D0: TPIS 1996 pt1 p97, pt2 p76.
 2 g10/98 B   1.00S   1.00    0.00    0.00    0.00 0   42.8770000     273519.405
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8724.105
-3.839490100D+04 6.989417490D+02-1.213980460D+00 1.396391264D-02-1.689881284D-05
 1.038889985D-08-2.582063989D-12               2.865685472D+04 3.154823443D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8724.105
 1.358760165D+06-4.364035960D+03 9.034307590D+00-2.114548699D-03 4.189275310D-07
-1.354787322D-11-1.360684605D-15               5.913065450D+04-3.336693370D+01
BS2             Cons & D0:TPIS 1996 pt1 p99, pt2 p77.
 2 g 9/98 B   1.00S   2.00    0.00    0.00    0.00 0   74.9430000      63867.460
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13559.560
 1.820264374D+04-5.150671890D+02 8.547515000D+00-1.626155268D-03 1.866387194D-06
-1.277165468D-09 3.681980690D-13               8.186839750D+03-1.778380851D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13559.560
 5.120402510D+05-1.938581076D+03 9.814873460D+00-1.339731606D-03 3.754301160D-07
-4.400383780D-11 1.887662968D-15               1.736535000D+04-2.757542709D+01
B2              Props & D0: TPIS 1996 pt1 p8, pt2 p7.
 2 g 9/98 B   2.00    0.00    0.00    0.00    0.00 0   21.6220000     857370.506
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8805.106
-1.516418096D+05 2.630168946D+03-1.381358321D+01 5.216225190D-02-6.930494740D-05
 4.469410390D-08-1.128496456D-11               8.995251050D+04 9.813118490D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8805.106
 1.094594495D+06-2.602735739D+03 6.909456210D+00-6.405949890D-04 1.951732355D-07
-2.555902119D-11 1.053557323D-15               1.187807611D+05-1.949045025D+01
B2C             Cons & D0:TPIS 1996 pt1 p110, pt2 p88.
 2 g 9/98 B   2.00C   1.00    0.00    0.00    0.00 0   33.6327000     800432.614
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11723.114
-4.166519870D+04 5.797779520D+02 1.411017091D+00 1.174705713D-02-1.066474425D-05
 4.717232620D-09-7.970013260D-13               9.196874200D+04 1.769254387D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11723.114
 1.159241019D+06-4.567798810D+03 1.228672097D+01-2.500830701D-03 6.409979850D-07
-6.932935770D-11 2.672933741D-15               1.222442137D+05-5.199066186D+01
B2CL4           Cons & Hf: TPIS 1996 pt1 p77 pt2 p54.
 2 g10/97 B   2.00CL  4.00    0.00    0.00    0.00 0  163.4328000    -490000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21588.132
 4.285555130D+04-7.280748810D+02 9.315763670D+00 2.331629623D-02-3.511247610D-05
 2.464057658D-08-6.735479960D-12              -5.819023240D+04-1.622084979D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21588.132
-6.427987030D+05 5.078562990D+02 1.486725022D+01 2.026983515D-06 6.272718810D-09
-1.218822573D-12 7.241208410D-17              -6.820066000D+04-4.139111770D+01
B2F4            Cons & Hf: TPIS 1996 pt1 p64 pt2 p41.
 2 g10/97 B   2.00F   4.00    0.00    0.00    0.00 0   97.6156128   -1438000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17680.793
-5.971695640D+04 8.189425440D+02-6.437671290D-01 3.858966070D-02-4.313053190D-05
 2.404463223D-08-5.393559350D-12              -1.790041225D+05 3.552179970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17680.793
 3.855865890D+04-2.928842655D+03 1.792063736D+01-9.523998270D-04 1.614708845D-07
-1.428613504D-11 5.218739670D-16              -1.613051924D+05-7.184803250D+01
B2H6            Cons & Hf: TPIS 1996 pt1 p37 pt2 p22.
 2 tpis96 B   2.00H   6.00    0.00    0.00    0.00 0   27.6696400      36600.000
```

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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12023.912
 1.926858874D+04 5.582852520D+02-6.217713640D+00 4.847406790D-02-4.518685150D-05
 2.520801926D-08-6.445712170D-12                 1.337427345D+03 5.271558140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12023.912
 2.852173433D+06-1.563259695D+04 3.222418640D+01-3.722582630D-03 7.681545020D-07
-8.370211270D-11 3.731199690D-15                 9.338411570D+04-1.915687257D+02
B2O             Cons & D0: TPIS 1996 pt1 p19, pt2 p14.
 2 g 9/98 B   2.00O   1.00    0.00    0.00    0.00 0   37.6214000     192798.018
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11783.018
-5.699546760D+04 1.018000465D+03-2.636481947D+00 2.746009279D-02-3.632432720D-05
 2.406890217D-08-6.384129720D-12                 1.703874394D+04 3.855346110D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11783.018
-1.628723220D+05-3.876289810D+02 7.787723520D+00-1.146822108D-04 2.528097612D-08
-2.893783941D-12 1.339210475D-16                 2.263035354D+04-1.908513011D+01
B2O2            Cons & Hf0: TPIS 1996 pt1 p19, pt2 p15.
 2 tpis96 B   2.00O   2.00    0.00    0.00    0.00 0   53.6208000    -457711.486
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13396.618
 8.174391690D+04-1.732702797D+03 1.605560926D+01-2.160057288D-02 3.566854570D-05
-2.660198794D-08 7.531833240D-12                -4.899632900D+04-6.172702390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13396.618
 4.605789660D+05-2.990079203D+03 1.256764079D+01-7.850974950D-04 1.672537624D-07
-1.867694780D-11 8.486190670D-16                -4.015748150D+04-4.874413710D+01
B2O3            Cons & Hsubl: TPIS 1996 pt1 p25 pt2 p18.
 2 tpis96 B   2.00O   3.00    0.00    0.00    0.00 0   69.6202000    -835382.271
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14418.729
 7.379611910D+04-1.263620592D+03 1.072681512D+01 3.841383720D-04 5.976058380D-06
-6.552891350D-09 2.123951064D-12                -9.628183140D+04-3.088078011D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14418.729
 3.905035300D+05-3.691348210D+03 1.555502598D+01-9.707645510D-04 2.068887872D-07
-2.310858356D-11 1.050136734D-15                -8.263054410D+04-6.390863440D+01
B2(OH)4         Cons & D0: TPIS 1996 pt1 p52 pt2 p33.
 2 g 9/98 B   2.00O   4.00H   4.00    0.00    0.00 0   89.6513600   -1254987.531
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19443.069
-1.728717249D+04 8.495913480D+02-8.715959570D+00 9.362362610D-02-1.278784165D-04
 8.813671160D-08-2.400605571D-11                -1.564337133D+05 7.120169310D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19443.069
 2.983925656D+06-1.207469577D+04 3.162610570D+01-5.163682440D-04-4.232093970D-08
 1.671977280D-11-1.156366726D-15                -8.280976970D+04-1.653010498D+02
B2S             Cons & D0:TPIS 1996 pt1 p100, pt2 p78.
 2 g 9/98 B   2.00S   1.00    0.00    0.00    0.00 0   53.6880000     622260.705
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13182.705
 6.638609300D+04-9.201185690D+02 8.699831340D+00 7.645589010D-04-3.709026030D-06
 3.642373980D-09-1.197766071D-12                 7.770375800D+04-2.251709650D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13182.705
-1.211501483D+05-6.473398450D+01 7.546825610D+00-1.820541450D-05 3.923951170D-09
-4.403862380D-13 2.003651718D-17                 7.258531870D+04-1.394968435D+01
B2S2            Cons & Hf0:TPIS 1996 pt1 p100, pt2 p79.
 2 tpis96 B   2.00S   2.00    0.00    0.00    0.00 0   85.7540000     138317.112
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14569.112
-7.061549970D+04 7.182944780D+02 1.919797788D+00 2.036407461D-02-2.309813846D-05
 1.311616725D-08-2.996394781D-12                 1.100829019D+04 1.855406084D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14569.112
-1.641535014D+05-7.742865640D+02 1.107731737D+01-2.313278554D-04 5.125614290D-08
-5.894081230D-12 2.738673834D-16                 1.733003515D+04-3.359763500D+01
B2S3            Cons & Hf0: TPIS 1996 pt1 p102 pt2 p81.
 2 tpis96 B   2.00S   3.00    0.00    0.00    0.00 0  117.8200000      17754.057
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19938.057
-3.431268500D+04 5.587615370D+02 3.414077410D+00 2.398333891D-02-2.841617637D-05
 1.690005199D-08-4.060070710D-12                -3.027690575D+03 1.846771683D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19938.057
-1.905855086D+05-9.348342480D+02 1.369333613D+01-2.766647250D-04 6.110155800D-08
-7.008048570D-12 3.249524620D-16                 2.906433760D+03-3.946866660D+01
B3N3H6          Borazole. Cons & Hf: TPIS 1996 pt1 p107 pt2 p85.
 2 tpis96 B   3.00N   3.00H   6.00    0.00    0.00 0   80.5008600    -512000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16221.348
-1.552621082D+05 4.010211270D+03-3.382491300D+01 1.624575582D-01-2.065528647D-04
 1.368862991D-07-3.673470900D-11                -8.051253400D+04 1.995000773D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16221.348
 3.739245170D+06-1.941238951D+04 4.445070030D+01-3.210308050D-03 5.717465420D-07
-5.486692140D-11 2.191943197D-15                 4.758426160D+04-2.641156603D+02
B3O3CL3         Cons & Hf0: TPIS 1996 pt1 p80 pt2 p57.
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 2 tpis96 B   3.00O   3.00CL  3.00    0.00    0.00 0  186.7893000   -1635982.041
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24451.781
-4.284452800D+04 1.005623966D+03-4.556519630D+00 8.117967140D-02-1.038385803D-04
 6.621422330D-08-1.695748504D-11                -2.040907277D+05 5.466113080D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24451.781
-7.414059810D+05-2.527447455D+03 2.687263667D+01-7.463389360D-04 1.646334110D-07
-1.886231553D-11 8.737926310D-16                -1.923509858D+05-1.185636327D+02
B3O3FCL2          Cons & Hf0: TPIS 1996 pt1 p89 pt2 p68.
 2 tpis96 B   3.00O   3.00F   1.00CL  2.00    0.00 0  170.3350032   -1883807.681
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23448.139
-3.719120070D+04 8.673745890D+02-4.095778460D+00 7.815563970D-02-9.767035170D-05
 6.097610090D-08-1.532880319D-11                -2.331383552D+05 5.198087630D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23448.139
-7.162360830D+05-2.851210308D+03 2.710953133D+01-8.400919640D-04 1.852318684D-07
-2.121694694D-11 9.827291560D-16                -2.202729252D+05-1.210679418D+02
B3O3F2CL          Cons & Hf0: TPIS 1996 pt1 p89 pt2 p67.
 2 tpis96 B   3.00O   3.00F   2.00CL  1.00    0.00 0  153.8807064   -2132816.827
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22260.991
-5.277015540D+04 1.104904696D+03-5.854181050D+00 7.953943100D-02-9.592660770D-05
 5.799856310D-08-1.416698348D-11                -2.640400115D+05 6.071246930D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22260.991
-6.810787490D+05-3.370009020D+03 2.748953579D+01-9.905442560D-04 2.182908440D-07
-2.499573480D-11 1.157532106D-15                -2.472114785D+05-1.261501577D+02
B3O3F3            Cons & Hf0: TPIS 1996 pt1 p67 pt2 p44.
 2 tpis96 B   3.00O   3.00F   3.00    0.00    0.00 0  137.4264096   -2382699.078
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21200.738
-7.251549780D+04 1.400996228D+03-7.906716200D+00 8.217161850D-02-9.633152660D-05
 5.668194260D-08-1.349024305D-11                -2.953461728D+05 7.001536830D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21200.738
-6.629822910D+05-3.784946870D+03 2.779526578D+01-1.112096232D-03 2.450806704D-07
-2.806484980D-11 1.299750466D-15                -2.748865475D+05-1.315605015D+02
Ba                TPIS 1996;NSRDS-NBS 35 1971;NSRDS-NBS 34 1970
 3 g10/97 BA  1.00    0.00    0.00    0.00    0.00 0  137.3270000     185000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 2.222563526D+03-3.407977850D+01 2.706751118D+00-6.382894490D-04 1.063003846D-06
-9.102624270D-10 3.148062219D-13                 2.166549702D+04 5.102545880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.926579228D+07 6.006501040D+04-6.633964130D+01 3.507565930D-02-7.807601830D-06
 8.085126800D-10-3.199486918D-14                -3.589663720D+05 5.007583400D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 3.483452070D+08-2.925558261D+05 9.774888490D+01-1.345477126D-02 9.567239790D-07
-3.380662310D-11 4.727390540D-16                 2.250335260D+06-7.968444410D+02
Ba+               NSRDS NBS 35 vIII 1971.
 3 g10/97 BA  1.00E  -1.00    0.00    0.00    0.00    0.00 0  137.3264514     694049.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-5.423167550D+04 6.744680780D+02-8.940272500D-01 8.796642950D-03-1.222812901D-05
 8.387953870D-09-2.037964358D-12                 7.941774640D+04 2.607063698D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 8.794971850D+06-1.951817883D+04 1.485542861D+01-9.404233500D-04-7.031257790D-07
 1.667412753D-10-1.070117310D-14                 2.146800732D+05-9.228264190D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.055569557D+08 4.530799570D+04-5.410673220D-01-7.531497600D-04 1.295568595D-07
-6.013388590D-12 8.846178515D-17                -3.000874708D+05 4.370610780D+01
BaBr              D0,Props:TPIS 1996 pt1 p576; pt2 p437.
 2 tpis96 BA  1.00BR  1.00    0.00    0.00    0.00 0  217.2310000     -75324.677
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10200.123
-6.912557440D+02-6.245500160D+01 4.796677650D+00-6.838004940D-04 1.043947680D-06
-7.441224300D-10 2.172187003D-13                -1.011349165D+04 5.196454870D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10200.123
-1.056014042D+06 1.034740207D+03 6.735729380D+00-3.784026300D-03 1.952196896D-06
-3.347831880D-10 1.893189803D-14                -1.950233645D+04-5.069279640D+00
BaBr2             Hsubl & cons: TPIS v3 pt1 p579; pt2 p439.
 2 tpis96 BA  1.00BR  2.00    0.00    0.00    0.00 0  297.1350000    -412514.741
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15485.759
-5.143374060D+03-3.870518460D+01 7.162446970D+00-3.696715310D-04 4.689715270D-07
-3.107902475D-10 8.363582050D-14                -5.153318260D+04 9.741407000D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15485.759
-8.928251210D+03-7.536558890D-01 7.000658210D+00-2.949821710D-07 7.092392110D-11
-8.670038100D-15 4.221742310D-19                -5.172669490D+04 1.910185706D+00
BaCL              D0,Probs:TPIS 1996 pt1 p570; pt2 p433.
 2 tpis96 BA  1.00CL  1.00    0.00    0.00    0.00 0  172.7797000    -136290.881
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9877.119
-2.661946867D+03-7.724996340D+01 4.746106050D+00-3.523548880D-04 3.999198350D-07
-1.936413749D-10 4.124048530D-14              -1.736328141D+04 3.904452480D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9877.119
-1.075410089D+06 1.209303069D+03 6.272558600D+00-3.288110310D-03 1.717751087D-06
-2.910607065D-10 1.632658438D-14              -2.779173737D+04-3.574187820D+00
BaCL+           D0,Estim.constants:TPIS 1996 pt1 p572; pt2 p434.
 2 g12/97 BA  1.00CL  1.00E  -1.00    0.00    0.00 0  172.7791514     348697.630
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9668.230
-8.951556690D+02-1.334692684D+02 4.935416120D+00-7.574054510D-04 8.355724000D-07
-4.685258510D-10 1.095343103D-13               4.125155990D+04 1.896275774D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9668.230
-1.829198157D+04-2.931616688D+00 4.502280710D+00 3.671788490D-05 2.396147871D-09
 5.479458600D-14 1.174342316D-18               4.055100150D+04 4.503762960D+00
BaCL2           Hsubl & cons: TPIS v3 pt1 p575; pt2 p436.
 2 tpis96 BA  1.00CL  2.00    0.00    0.00    0.00 0  208.2324000    -499301.387
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14599.113
-1.157501999D+03-2.054518828D+02 7.837514050D+00-1.867700704D-03 2.335378734D-06
-1.531373341D-09 4.088525090D-13              -6.115665280D+04-5.978153540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14599.113
-2.216598768D+04-4.002483810D+00 7.003426740D+00-1.515820808D-06 3.611849210D-10
-4.386759060D-14 2.125803293D-18              -6.219095270D+04-1.132444016D+00
BaF             D0,Probs:TPIS 1996 pt1 p562; pt2 p429.
 2 tpis96 BA  1.00F   1.00    0.00    0.00    0.00 0  156.3254032    -318993.788
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9342.112
 2.530317292D+04-4.716995100D+02 6.185036220D+00-3.366678800D-03 4.011834560D-06
-2.506578601D-09 6.477258160D-13              -3.731872140D+04-6.220715380D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9342.112
 1.868380434D+06-7.071099600D+03 1.466959284D+01-6.995950200D-03 2.366313845D-06
-3.287734300D-10 1.647896238D-14               3.571780680D+03-6.662390920D+01
BaF+            D0,Estim.constants:TPIS 1996 pt1 p566; pt2 p430.
 2 g12/97 BA  1.00F   1.00E  -1.00    0.00    0.00 0  156.3248546     134063.214
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9201.714
 2.840719922D+04-4.863571820D+02 5.946058390D+00-2.429844077D-03 2.445346729D-06
-1.316757471D-09 2.974886320D-13               1.730639076D+04-5.951206930D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9201.714
-4.054423670D+04-1.701997704D+01 4.513055340D+00 2.632753508D-05 2.612088236D-09
-9.502197930D-14 6.515176160D-18               1.474486570D+04 2.783167711D+00
BaF2            Hsubl & cons: TPIS v3 pt1 p569; pt2 p432.
 2 tpis96 BA  1.00F   2.00    0.00    0.00    0.00 0  175.3238064    -812003.483
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13437.017
 3.488395520D+04-7.648459560D+02 9.797750380D+00-5.756457510D-03 6.775603800D-06
-4.243614750D-09 1.093687692D-12              -9.590356450D+04-2.082035292D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13437.017
-5.508633660D+04-1.691114228D+01 7.013564880D+00-5.731909770D-06 1.321203959D-09
-1.565528167D-13 7.444983020D-18              -9.983529700D+04-4.389581490D+00
BaH             D0,Props:TPIS 1996 pt1 p554; pt2 p423.
 2 tpis96 BA  1.00H   1.00    0.00    0.00    0.00 0  138.3349400     209535.105
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8731.105
-3.765268880D+04 6.986680120D+02-1.313524351D+00 1.460648882D-02-1.802974829D-05
 1.133031115D-08-2.865589059D-12               2.097478889D+04 3.230802600D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8731.105
-6.755466570D+06 1.730700212D+04-1.136812458D+01 5.617744740D-03-3.180788850D-07
-1.052342502D-10 1.111101879D-14              -8.954070380D+04 1.182377538D+02
BaI             D0,Props:TPIS 1996 pt1 p581; pt2 p440.
 2 tpis96 BA  1.00I   1.00    0.00    0.00    0.00 0  264.2314700     -10237.675
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10397.125
-4.186285540D+03 1.033094613D+01 4.428900230D+00 3.026019976D-04-2.591429408D-07
 1.741605400D-10-3.370062760D-14              -2.636169733D+03 8.201924680D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10397.125
-3.533859660D+06 7.394258000D+03 1.285151488D+00-2.303429302D-03 2.214839289D-06
-4.681096810D-10 3.011371472D-14              -5.340229590D+04 3.710443870D+01
BaI2            Hsubl & cons: TPIS v3 pt1 p584; pt2 p442.
 2 tpis96 BA  1.00I   2.00    0.00    0.00    0.00 0  391.1359400    -288439.965
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15790.435
-4.241592730D+03-1.862214382D+01 7.078556750D+00-1.793922821D-04 2.281437677D-07
-1.514647881D-10 4.081498360D-14              -3.670351490D+04 3.163138970D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15790.435
-6.048224800D+03-3.622729450D-01 7.000317450D+00-1.425793502D-07 3.433349420D-11
-4.201754980D-15 2.047703474D-19              -3.679650750D+04 3.615475320D+00
BaO             Hsubl,Props(extrap):TPIS 1996 pt1 p550; pt2 p419.
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 3 tpis96 BA  1.00O   1.00    0.00    0.00    0.00 0  153.3264000    -117948.392
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9014.108
 3.764398500D+04-5.071555300D+02 5.392847280D+00-4.119324690D-04-6.527896620D-07
 9.430588420D-10-3.436603030D-13                -1.275552614D+04-3.752213760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9014.108
 1.318481698D+07-3.854253250D+04 4.686741610D+01-2.188646633D-02 5.335677450D-06
-5.152304300D-10 1.433083400D-14                2.306902396D+05-3.028332772D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9014.108
-1.104748482D+09 3.561451690D+05-1.236258085D+01-2.812895475D-03 3.310897210D-07
-1.254960778D-11 1.696392420D-16               -3.157682531D+06 2.067297489D+02
BaO+            D0,Estim.cons:TPIS 1996 pt1 p552; pt2 p421.
 3 g11/98 BA  1.00O   1.00E  -1.00    0.00    0.00 0  153.3258514     511704.686
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9469.786
 3.566410970D+05-3.779246710D+03 1.673544137D+01-1.306611610D-02 2.686157445D-06
 4.044077950D-09-2.016508813D-12                7.983268490D+04-7.285118550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9469.786
-3.317679230D+05 1.594253495D+03 3.227247810D+00 5.722641500D-04-1.147415658D-07
 1.382873231D-11-6.384437030D-16                5.025247610D+04 1.409092365D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9469.786
-3.283193020D+06 2.046049762D+03 4.048225140D+00 9.872145390D-05 7.763808620D-11
 2.536329860D-13-1.334411326D-18                4.456858530D+04 8.528620900D+00
BaOH            Hf0 & cons: TPIS v3 pt1 p557; pt2 p425.
 2 tpis96 BA  1.00O   1.00H   1.00    0.00    0.00 0  154.3343400    -224256.513
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11224.581
 3.776231510D+04-8.891390220D+02 9.531718000D+00-5.458825900D-03 4.941783010D-06
-1.809327537D-09 2.050048305D-13               -2.441852965D+04-2.489410158D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11224.581
 2.637336694D+06-8.365410400D+03 1.599803975D+01-5.098446050D-03 1.594657431D-06
-2.180478542D-10 1.084610688D-14                2.393550647D+04-7.490705790D+01
BaOH+           Hf0 & cons: TPIS v3 pt1 p558; pt2 p426.
 2 tpis96 BA  1.00O   1.00H   1.00E  -1.00    0.00 0  154.3337914     202019.313
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11302.980
 2.797632165D+04-7.680769400D+02 9.052978440D+00-4.368577900D-03 3.523497260D-06
-8.386360870D-10-6.475457470D-14                2.623280802D+04-2.264561641D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11302.980
 8.766738430D+05-2.335819600D+03 7.973166060D+00 1.038679898D-04-6.319485780D-08
 1.028729445D-11-5.741808570D-16                3.772517470D+04-1.930805001D+01
Ba(OH)2         Hf0 & cons: TPIS v3 pt1 p561; pt2 p428.
 2 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 0  171.3416800    -606666.472
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17388.725
 5.702814900D+04-1.577384797D+03 1.659935325D+01-1.039598275D-02 9.664889600D-06
-3.673621440D-09 4.625784990D-13               -6.835158900D+04-5.851911700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17388.725
 1.762908112D+06-4.676205420D+03 1.395135494D+01 2.051842928D-04-1.257265530D-07
 2.048917625D-11-1.144045777D-15               -4.545964410D+04-4.929457190D+01
BaS             D0,TabData:TPIS 1996 pt1 p585; pt2 p444.
 2 tpis96 BA  1.00S   1.00    0.00    0.00    0.00 0  169.3930000      38871.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9556.115
 1.377075147D+04-3.293500560D+02 5.811545840D+00-2.848973760D-03 3.576336020D-06
-2.325649347D-09 6.172805310D-13                4.964432450D+03-3.497953760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9556.115
 6.104262070D+06-2.227617479D+04 3.597513510D+01-2.157793740D-02 7.319872350D-06
-1.089038636D-09 5.884101950D-14                1.404138006D+05-2.141776242D+02
Ba2             D0,tabdata:Gurvich TPIS 1996 pt1 p545; pt2 p417.
 2 tpis96 BA  2.00    0.00    0.00    0.00    0.00 0  274.6540000     355964.337
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11359.137
-1.294177083D+04-7.276330080D+02 1.464866569D+01-3.966331650D-02 5.898711060D-05
-4.235300560D-08 1.189594362D-11                4.386712230D+04-4.145673670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11359.137
 2.160114547D+05 1.950676877D+02 2.253699771D+00 1.507750613D-04-4.742515000D-08
 7.048951960D-12-3.547440170D-16                4.167762970D+04 2.375906459D+01
Be              Hf:CODATA1989. JPCRD v26 n5 1997 p1185.
 3 g11/97 BE  1.00    0.00    0.00    0.00    0.00 0    9.0121820     324000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-4.112901520D-04 5.364967360D-06 2.499999972D+00 7.569203690D-11-1.097852652D-13
 8.002110240D-17-2.303022777D-20                3.822264590D+04 2.146172983D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-6.926285840D+05 2.466773005D+03-9.776613340D-01 2.458939515D-03-9.047950420D-07
 1.587880407D-10-9.415600603D-15                2.300212917D+04 2.623234754D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.145833520D+08-2.254147519D+05 4.411437910D+01-3.022853591D-03 1.178346131D-07
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-2.273387650D-12 1.196838345D-17                1.866686325D+06-3.752337400D+02
Be+             Spec: NSRDS-NBS 35 1971; NSRDS-NBS 34 1970.
 3 g 1/98 BE  1.00E  -1.00    0.00    0.00    0.00 0    9.0116334    1229701.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.471528569D+05 2.839228698D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-9.478135980D+04 2.768325398D+02 2.191388413D+00 1.648824289D-04-4.280166820D-08
 4.542350470D-12-6.270417825D-17                1.453850986D+05 5.055503840D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.152447735D+08 1.430568120D+05-3.438209900D+01 4.568436290D-03-2.777202671D-07
 8.414520880D-12-9.930107101D-17               -9.766963440D+05 3.215758390D+02
Be++            Moore: NSRDS-NBS 34 1970.
 3 g 3/97 BE  1.00E  -2.00    0.00    0.00    0.00 0    9.0110848    2993001.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.592279160D+05 2.145990203D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.592279160D+05 2.145990203D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.592279160D+05 2.145990203D+00
BeBO2           JANAF 6/66 JPCRD v14 sup 1 1985.
 2 J 6/66 BE  1.00B   1.00O   2.00    0.00    0.00 0   51.8219820    -482003.114
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.006912000D+00 1.804482400D-02-1.691758100D-05
 6.086537300D-09-1.727628500D-13               -5.923419700D+04 1.580555710D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.910837600D+00 3.266868400D-03-1.367812000D-06
 2.557621100D-10-1.772774100D-14               -6.050571500D+04-9.161658050D+00
BeBr            Props,D0: TPIS 1996 pt1 p374, pt2 p300.
 2 tpis96 BE  1.00BR  1.00    0.00    0.00    0.00 0   88.9161820     132446.308
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8971.108
 3.746288060D+04-4.722339070D+02 5.039409040D+00 5.798853220D-04-1.937634343D-06
 1.793372625D-09-5.672295580D-13                1.723135679D+04-2.573912886D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8971.108
 8.217238140D+05-2.850509348D+03 8.017266020D+00-2.105663212D-03 6.849136340D-07
-9.989129320D-11 5.192456840D-15                3.229372870D+04-2.326810811D+01
BeBr2           Hsubl & cons: TPIS v3 pt1 p377; pt2 p302.
 2 tpis96 BE  1.00BR  2.00    0.00    0.00    0.00 0  168.8201820    -234062.499
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12837.501
-2.118698678D+04 2.090382611D+02 3.731171310D+00 1.115501549D-02-1.542821761D-05
 1.052354444D-08-2.850006057D-12               -3.090456277D+04 9.458917720D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12837.501
-1.041331811D+05-1.543443092D+02 7.614465410D+00-4.556700630D-05 1.003180548D-08
-1.146879501D-12 5.301795380D-17               -2.984527608D+04-1.149360980D+01
BeCL            Props & D0: TPIS 1996 pt1 p369, pt2 p295.
 2 tpis96 BE  1.00CL  1.00    0.00    0.00    0.00 0   44.4648820      56693.107
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8861.107
 2.016138947D+04-1.413988978D+02 2.898223773D+00 6.069925510D-03-9.162038470D-06
 6.612620660D-09-1.859126853D-12                6.626691440D+03 7.900170930D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8861.107
 2.808845146D+05-1.103100122D+03 5.671189830D+00-5.443000450D-04 1.459036606D-07
-1.230971735D-11 9.900804760D-17                1.224649804D+04-8.382381490D+00
BeCL+           JANAF 6/68 JPCRD v14 sup 1 1985.
 2 J 6/68 BE  1.00CL  1.00E  -1.00    0.00    0.00 0   44.4643334     979083.090
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.896598400D+00 5.126749200D-03-6.442791100D-06
 3.563264000D-09-6.592508800D-13                1.167146600D+05 7.837270450D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.382750000D+00-1.847119800D-03 1.112368300D-06
-1.695299400D-10 6.100709100D-15                1.159971700D+05-5.062241350D+00
BeCLF           JANAF 6/65 JPCRD v14 sup 1 1985.
 2 J 6/65 BE  1.00CL  1.00F   1.00    0.00    0.00 0   63.4632852    -573191.974
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.102438100D+00 8.501749000D-03-8.909396300D-06
 4.007623200D-09-5.162753900D-13               -7.046873600D+04 4.099162810D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.440279100D+00 1.146369300D-03-4.854536000D-07
 9.128786500D-11-6.344354900D-15               -7.105977100D+04-7.728699690D+00
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BeCL2           Hsubl & cons: TPIS v3 pt1 p373; pt2 p298.
 2 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 0   79.9175820    -361539.140
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12080.860
-2.229957657D+04 1.528781667D+02 3.714994710D+00 1.067776550D-02-1.397766942D-05
 9.066693560D-09-2.350292311D-12              -4.590428230D+04 6.682544310D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12080.860
-1.154087460D+05-2.484300053D+02 7.685672140D+00-7.444960370D-05 1.649479787D-08
-1.895997075D-12 8.804973950D-17              -4.468747280D+04-1.500338533D+01
BeF             Props & D0: TPIS 1996 pt1 p363, pt2 p291.
 2 tpis96 BE  1.00F   1.00    0.00    0.00    0.00 0   28.0105852    -170624.795
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8711.105
-4.664497230D+04 7.887178850D+02-1.463363201D+00 1.381790494D-02-1.591299964D-05
 9.352931520D-09-2.229211181D-12              -2.522627476D+04 3.197634300D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8711.105
-1.857941543D+05 4.776082770D+01 4.269986020D+00 2.310668473D-04-6.657214920D-08
 1.152149888D-11-6.335586440D-16              -2.257950960D+04-2.184787270D-01
BeF2            Hsubl & cons: TPIS v3 pt1 p366; pt2 p293.
 2 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 0   47.0089884    -796588.236
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10879.764
 7.490270240D+03-2.878053102D+02 5.434712820D+00 3.903233460D-03-2.214865601D-06
-1.965806119D-10 4.042362270D-13              -9.591615640D+04-5.616616920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10879.764
-6.482018070D+04-7.684556060D+02 8.062860840D+00-2.227502549D-04 4.891598660D-08
-5.587886720D-12 2.583409761D-16              -9.395495490D+04-2.125660266D+01
BeH             Props,D0: TPIS 1996 pt1 p356, pt2 p286.
 2 tpis96 BE  1.00H   1.00    0.00    0.00    0.00 0   10.0201220     342252.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8648.104
-1.615149125D+03-5.935286080D+01 4.507269100D+00-5.264189610D-03 1.145319967D-05
-9.247883590D-09 2.700364753D-12               4.030193040D+04-3.485117050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8648.104
-2.424081636D+06 6.597398460D+03-3.626316480D+00 4.579634350D-03-1.163329056D-06
 1.297785691D-10-5.291885810D-15              -2.489846221D+03 5.216018690D+01
BeH+            JPCRD 1985 sup1 v14 pt1 p384.
 3 j 9/66 BE  1.00H   1.00E  -1.00    0.00    0.00 0   10.0195734    1178218.951
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8643.951
-3.220611020D+04 2.520229596D+02 3.207719570D+00-2.191287290D-03 6.902534490D-06
-5.769522630D-09 1.656414969D-12               1.392530660D+05 3.307044770D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8643.951
 4.622341590D+05-1.760169629D+03 5.379905550D+00 2.742462444D-05-1.167208170D-07
 3.557177910D-11-2.569695765D-15               1.515859734D+05-1.369222641D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8643.951
 2.266459986D+08-1.207646511D+05 2.630824847D+01-1.402096449D-03 3.760829760D-08
 6.342806240D-14-1.264548978D-17               1.121142116D+06-2.049239740D+02
BeH2            JPCRD 1985 sup1 v14 pt1 p387.
 2 j12/60 BE  1.00H   2.00    0.00    0.00    0.00 0   11.0280620     125520.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8732.228
-1.302458357D+05 1.920406347D+03-6.672382780D+00 2.192656183D-02-1.425445050D-05
 2.838301107D-09 4.618792600D-13               4.852866340D+03 5.861628420D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8732.228
 4.337793920D+05-3.572026530D+03 1.000577620D+01-9.619511580D-04 2.066582074D-07
-2.322739893D-11 1.060748507D-15               3.411054750D+04-4.507577070D+01
BeI             Props,D0: TPIS 1996 pt1 p378, pt2 p303.
 2 tpis96 BE  1.00I   1.00    0.00    0.00    0.00 0  135.9166520     207454.309
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9089.109
 3.530054810D+04-5.190950260D+02 5.714505240D+00-1.409073640D-03 7.664772120D-07
-2.601945105D-11-8.230960640D-14               2.637903657D+04-5.140997840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9089.109
-5.328206620D+05 1.139497861D+03 3.629171660D+00 1.704033769D-04 1.067048688D-07
-3.589457880D-11 2.722769560D-15               1.585474307D+04 9.370951270D+00
BeI2            Hsubl & cons: TPIS v3 pt1 p380; pt2 p305.
 2 tpis96 BE  1.00I   2.00    0.00    0.00    0.00 0  262.8211220     -64759.451
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13440.549
 3.592726180D+02-4.866059010D+01 5.241571180D+00 7.830305060D-03-1.169525374D-05
 8.389583910D-09-2.356636003D-12              -9.333220920D+03 2.896318281D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13440.549
-9.392372840D+04-8.959214380D+01 7.565554790D+00-2.577727326D-05 5.614265330D-09
-6.359663850D-13 2.917080336D-17              -9.814768620D+03-9.032042810D+00
BeN             JPCRD 1985 sup1 v14 pt1 p396.
 2 j 6/63 BE  1.00N   1.00    0.00    0.00    0.00 0   23.0189220     427000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8725.221
-4.247783630D+04 7.590188900D+02-1.561469235D+00 1.496945721D-02-1.835608880D-05
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 1.146861461D-08-2.897470581D-12                4.683003320D+04 3.256974020D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8725.221
-5.909696160D+04-3.078649431D+02 4.727959150D+00-3.928158830D-05 2.006201069D-08
-2.300018068D-12 1.066101831D-16                5.156095710D+04-3.031378018D+00
BeO             Props & D0: TPIS 1996 pt1 p351, pt2 p280.
 3 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 0   25.0115820     128940.304
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8688.104
-4.869458320D+04 7.213473620D+02-3.784157320D-01 8.792203850D-03-7.070151260D-06
 2.250175620D-09-2.799117872D-14                1.101466639D+04 2.574081184D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8688.104
-3.503472450D+07 1.055859473D+05-1.165011722D+02 6.477369480D-02-1.649656058D-05
 2.005558400D-09-9.426891790D-14               -6.570018000D+05 8.640898030D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8688.104
-7.440106320D+07 4.309665300D+04-1.019586064D-01 2.617209088D-04-2.461810861D-08
 1.124733698D-12-1.832802285D-17               -3.402379380D+05 4.487040230D+01
BeOH            Hf0 & cons: TPIS v3 pt1 p358; pt2 p288.
 2 tpis96 BE  1.00O   1.00H   1.00    0.00    0.00 0   26.0195220     -99717.721
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10798.450
-3.853024520D+04 4.498059290D+02 1.532096459D+00 1.299912603D-02-1.708979996D-05
 1.169968182D-08-3.163183710D-12               -1.559046567D+04 1.545542930D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10798.450
 8.550330310D+05-2.646537838D+03 8.204784630D+00 1.110814513D-05-4.265364000D-08
 7.926511920D-12-4.645419520D-16                3.121216271D+03-2.571641308D+01
BeOH+           JPCRD 1985 sup1 v14 pt1 p386.
 3 j12/75 BE  1.00O   1.00H   1.00E  -1.00    0.00 0   26.0189734     759983.920
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9550.904
 7.106119160D+04-8.068981600D+02 5.603107810D+00 4.932070860D-03-7.722847160D-06
 5.910889810D-09-1.695201901D-12 0.000000000D+00 9.440782420D+04-1.088099852D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9550.904
 8.134874390D+05-2.814653683D+03 8.381145010D+00-6.942073280D-05-2.369535806D-08
 5.678106380D-12-3.583253560D-16 0.000000000D+00 1.073129932D+05-2.901093335D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9550.904
-6.279111750D+06 2.090044240D+03 7.025559910D+00 5.492111300D-05-3.446137200D-09
 1.115947764D-13-1.461494242D-18 0.000000000D+00 6.914837000D+04-1.732443156D+01
Be(OH)2         Hf0: TPIS v3 pt1 p360; pt2 p290.
 2 tpis96 BE  1.00O   2.00H   2.00    0.00    0.00 0   43.0268620    -638864.416
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15225.858
 7.863089830D+03-7.397142250D+02 1.043303334D+01 4.514249530D-03-6.950601530D-06
 5.777030040D-09-1.727199382D-12               -7.585676960D+04-3.301466610D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15225.858
 1.722889403D+06-5.242477190D+03 1.486877785D+01 3.931498360D-05-8.920276310D-08
 1.630912925D-11-9.505371140D-16               -4.642823840D+04-6.476804020D+01
BeS             Props & D0: TPIS 1996 pt1 p381, pt2 p307.
 2 tpis96 BE  1.00S   1.00    0.00    0.00    0.00 0   41.0781820     247095.306
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8780.106
-7.390579080D+03 2.828134792D+02 6.552019400D-01 1.076012495D-02-1.398380157D-05
 8.818418890D-09-2.110588578D-12                2.751593294D+04 1.980497213D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8780.106
-1.655708361D+07 5.431466120D+04-6.351859250D+01 3.964091990D-02-1.078978696D-05
 1.394030343D-09-6.936955040D-14               -3.121559628D+05 4.803455300D+02
Be2             D0,Props(extrp): TPIS 1996 pt1 p346 pt2 p277.
 2 tpis96 BE  2.00    0.00    0.00    0.00    0.00 0   18.0243640     637543.318
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9838.118
-1.580873810D+05 2.035567774D+03-3.691580630D+00 1.028818435D-02-9.603854510D-06
 4.707519420D-09-9.374688790D-13                6.526968370D+04 4.879324990D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9838.118
 1.010034484D+05 1.414207488D+02 2.292070182D+00 1.543331824D-04-5.801043000D-08
 1.003129697D-11-5.682818340D-16                7.550139730D+04 1.238758616D+01
Be2CL4          Hf0: TPIS v3 pt1 p374; pt2 p299.
 2 tpis96 BE  2.00CL  4.00    0.00    0.00    0.00 0  159.8351640    -819604.973
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22641.384
 1.216152589D+05-2.000824823D+03 1.723384275D+01 5.810448280D-03-1.362970089D-05
 1.156602362D-08-3.552255800D-12               -9.206475470D+04-6.137960900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22641.384
-3.354920080D+05-2.316199283D+02 1.617047912D+01-6.734405950D-05 1.472073032D-08
-1.672352806D-12 7.688773970D-17               -1.031075197D+05-5.047010500D+01
Be2F4           Hf0: TPIS v3 pt1 p368; pt2 p294.
 2 tpis96 BE  2.00F   4.00    0.00    0.00    0.00 0   94.0179768   -1731699.842
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19834.508
-6.327701870D+03-6.902533720D+01 5.470937230D+00 3.097341347D-02-4.094310060D-05
 2.668113685D-08-6.942909560D-12               -2.105979269D+05-2.073546195D-01
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19834.508
-3.681834950D+05-9.439191480D+02 1.670099855D+01-2.797974015D-04 6.178061720D-08
-7.083080190D-12 3.282791040D-16              -2.089045725D+05-6.092665760D+01
Be2O            Hf0 & cons: TPIS v3 pt1 p353; pt2 p282.
 2 tpis96 BE  2.00O   1.00    0.00    0.00    0.00 0   34.0237640    -37033.803
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11190.386
-4.263673570D+02-1.159556261D+02 4.082677770D+00 1.015885064D-02-1.326015538D-05
 8.488955360D-09-2.168039077D-12              -5.362258120D+03 1.253737886D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11190.386
-1.412646378D+05-3.498644590D+02 7.760932680D+00-1.044953518D-04 2.313342334D-08
-2.657722263D-12 1.233820439D-16              -5.172385490D+03-1.854887619D+01
Be2OF2
 2 J 6/66 BE  2.00O   1.00F   2.00    0.00    0.00 0   72.0205704   -1204597.761
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.860002600D+00 1.943898200D-02-1.881876000D-05
 7.100950300D-09-3.722525800D-13              -1.470395900D+05 3.241733410D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 1.031134300D+01 2.925815100D-03-1.248198700D-06
 2.365216900D-10-1.655916000D-14              -1.484462300D+05-2.448768300D+01
Be2O2           Hf0: TPIS v3 pt1 p354; pt2 p283.
 2 tpis96 BE  2.00O   2.00    0.00    0.00    0.00 0   50.0231640    -411635.309
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10928.932
-3.031719530D+04 1.163353177D+03-8.733155950D+00 5.372002930D-02-7.279439190D-05
 4.894928250D-08-1.312147056D-11              -5.546936880D+04 6.953282640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10928.932
-3.960576640D+05-9.074948830D+02 1.067160422D+01-2.670905218D-04 5.877629990D-08
-6.718664090D-12 3.105949075D-16              -4.861114330D+04-3.616546890D+01
Be3O3           Hf0: TPIS v3 pt1 p355; pt2 p284.
 2 tpis96 BE  3.00O   3.00    0.00    0.00    0.00 0   75.0347460   -1023720.628
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15125.733
-2.738072346D+04 8.743832600D+02-6.599606120D+00 6.533021140D-02-8.762305740D-05
 5.817244790D-08-1.540600500D-11              -1.284679012D+05 5.837203120D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15125.733
-5.890809360D+05-1.392823588D+03 1.703450699D+01-4.127330740D-04 9.107529150D-08
-1.043465231D-11 4.833053770D-16              -1.219045534D+05-7.000614510D+01
Be4O4           Hf0: TPIS v3 pt1 p356; pt2 p285.
 2 tpis96 BE  4.00O   4.00    0.00    0.00    0.00 0  100.0463280   -1649294.582
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15833.899
-6.893255640D+04 1.687565069D+03-1.479616594D+01 1.007319774D-01-1.291057622D-04
 8.243136760D-08-2.111283987D-11              -2.072877151D+05 1.002507262D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15833.899
-8.841338460D+05-2.726394165D+03 2.402941774D+01-8.114675460D-04 1.794255972D-07
-2.059359498D-11 9.552905330D-16              -1.923710587D+05-1.136620750D+02
Br              Hf:CODATA1989. NSRDS-NBS 35 vII 1971;NSRDS-NBS 34 1970.
 3 g 3/97 BR  1.00    0.00    0.00    0.00    0.00 0   79.9040000    111870.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-3.700294130D+03 6.145215680D+01 2.092120709D+00 1.376818901D-03-2.445566706D-06
 2.050975203D-09-5.144249259D-13               1.242508646D+04 8.996166270D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-4.789717210D+06 1.692051943D+04-2.024085287D+01 1.395620311D-02-3.656230430D-06
 4.489780820D-10-2.122507430D-14              -9.207054610D+04 1.661695880D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.122781277D+08 6.345962000D+04-8.617874270D+00 1.180126568D-03-6.219227900D-08
 1.741185523D-12-2.094677726D-17              -5.014640180D+05 1.086136282D+02
Br+             Spec: NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g10/97 BR  1.00E  -1.00    0.00    0.00    0.00 0   79.9034514    1257927.034
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.434
 3.981187420D+04-4.751581470D+02 4.734578980D+00-5.169324790D-03 5.905857520D-06
-2.885129283D-09 5.054894290D-13               1.529052046D+05-5.769283220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.434
 1.741149829D+06-5.455465670D+03 8.470663350D+00-2.683465574D-03 6.590454560D-07
-7.953770300D-11 3.735898818D-15               1.851781643D+05-3.637909030D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.434
-6.174903280D+07 3.641704160D+04-5.739744680D+00 1.067497350D-03-7.127689890D-08
 2.155618820D-12-1.769476126D-17              -1.399767498D+05 7.931577700D+01
Br-             JPCRD v14 n3 1985 p731.
 3 g10/97 BR  1.00E   1.00    0.00    0.00    0.00 0   79.9045486    -219000.472
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.708492743D+04 5.419556170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
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 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.708492743D+04 5.419556170D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.708492743D+04 5.419556170D+00
BrCL            TPIS 1989 v1 pt1 p213; pt2 p112.
 2 tpis89 BR  1.00CL  1.00    0.00    0.00    0.00 0  115.3567000      14789.113
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9407.113
 1.653291583D+04-3.578769280D+02 5.700622160D+00-2.201257188D-03 2.415146969D-06
-1.371032976D-09 3.227803420D-13                2.252619279D+03-4.155663570D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9407.113
-1.284863067D+05-1.138379626D+03 7.964040800D+00-3.438056670D-03 1.524999514D-06
-2.761469114D-10 1.694450407D-14                5.938264260D+03-1.925044779D+01
BrF             TPIS 1989 v1 pt1 p208; pt2 p109.
 2 tpis89 BR  1.00F   1.00    0.00    0.00    0.00 0   98.9024032     -58851.445
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9021.108
 3.836143190D+04-5.184611970D+02 5.458327050D+00-5.656843100D-04-4.121311970D-07
 7.859913480D-10-3.036161520D-13                -5.595539910D+03-4.901129500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9021.108
 3.771388470D+06-1.267493430D+04 2.080555930D+01-1.026359360D-02 3.308203590D-06
-4.903192250D-10 2.648275080D-14                7.062609720D+04-1.130253600D+02
BrF3            TPIS 1989 v1 pt1 p211; pt2 p110.
 2 tpis89 BR  1.00F   3.00    0.00    0.00    0.00 0  136.8992096    -255600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14711.620
 1.116455127D+05-1.959424330D+03 1.526220126D+01-7.999362300D-03 6.982030260D-06
-3.242757960D-09 6.164751460D-13                -2.345341551D+04-5.522633600D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14711.620
-1.886532240D+05-8.245232970D+01 1.006180694D+01-2.477319092D-05 5.478576860D-09
-6.282655260D-13 2.910628214D-17                -3.386800370D+04-2.298937369D+01
BrF5            TPIS 1989 v1 pt1 p212; pt2 p111.
 2 tpis89 BR  1.00F   5.00    0.00    0.00    0.00 0  174.8960160    -428800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19174.543
 2.211366805D+05-4.024809220D+03 2.734900212D+01-1.832254979D-02 1.721754649D-05
-8.753508630D-09 1.860196959D-12                -3.537447670D+04-1.244296466D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19174.543
-3.757647640D+05-1.575896472D+02 1.611869838D+01-4.776497800D-05 1.059755365D-08
-1.218527723D-12 5.657535450D-17                -5.667266800D+04-5.540839310D+01
BrO             Hf298,TabData:JPCRD 1996 v25 n4 p1069.
 2 j 3/96 BR  1.00O   1.00    0.00    0.00    0.00 0   95.9034000     125800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9061.000
 1.455431116D+04 1.225152439D+02-3.058728672D-01 2.117309202D-02-3.494261190D-05
 2.622639719D-08-7.508059540D-12                1.389149932D+04 2.527867438D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9061.000
-2.392612795D+06 6.932793130D+03-2.513183892D+00 3.446544560D-03-7.569536840D-07
 6.514291340D-11-1.715768736D-15                -3.084499064D+04 5.361048360D+01
OBrO            JPCRD 1996 v25 n4 p1069.
 2 j 3/96 BR  1.00O   2.00    0.00    0.00    0.00 0  111.9028000     151954.526
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11394.630
 3.470213230D+04-3.401341820D+02 3.932251620D+00 1.215938586D-02-1.901501702D-05
 1.398631495D-08-3.992899760D-12                1.875955788D+04 6.361235180D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11394.630
-1.624504660D+05-1.453689372D+02 7.105822130D+00-4.141362070D-05 8.981833260D-09
-1.013712869D-12 4.635133140D-17                1.650075386D+04-9.111817920D+00
BrOO            JPCRD 1996 v25 n4 p1069.
 2 j 3/96 BR  1.00O   2.00    0.00    0.00    0.00 0  111.9028000     108000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12850.660
-4.417619900D+04 4.959637160D+02 3.239884950D+00 5.941502110D-03-3.402696770D-06
-3.444778160D-11 4.811957950D-13                8.815221980D+03 1.607446878D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12850.660
 6.172483480D+03-6.585049660D+02 7.483955330D+00-1.920530746D-04 4.226946170D-08
-4.837392610D-12 2.239741320D-16                1.460353470D+04-9.850380240D+00
BrO3            JPCRD 1996 v25 n4 p1069.
 2 j 3/96 BR  1.00O   3.00    0.00    0.00    0.00 0  127.9022000     220820.685
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13100.841
 1.063901881D+05-1.501928813D+03 9.703657430D+00 8.133000760D-03-1.531857845D-05
 1.199117619D-08-3.512747870D-12                3.233135990D+04-2.735125430D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13100.841
-2.822851113D+05-2.358973461D+02 1.017525279D+01-6.978451050D-05 1.535701661D-08
-1.754454950D-12 8.104100150D-17                2.401140140D+04-2.588197197D+01
Br2             TPIS 1989 v1 pt1 p200; pt2 p104.
 2 tpis89 BR  2.00    0.00    0.00    0.00    0.00 0  159.8080000      30910.000
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9725.117
 7.497047540D+03-2.350884557D+02 5.491934320D+00-2.227573303D-03 2.932401703D-06
-1.954889514D-09 5.312307890D-13                3.521475050D+03-1.964151570D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9725.117
-4.311698570D+06 1.111268634D+04-5.555775610D+00 3.630516590D-03-2.754164226D-07
-6.217506760D-11 7.375341620D-15               -7.036584160D+04 7.878478020D+01
BrBrO           Hform,Cons: JPCRD 1996 v25 n4 p1069.
 2 j 3/96 BR  2.00O   1.00    0.00    0.00    0.00 0  175.8074000     168000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13137.498
 1.617498037D+04-2.464406776D+02 5.912858450D+00 4.980354280D-03-8.099958250D-06
 6.072776260D-09-1.753715313D-12                1.974012093D+04 2.009704963D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13137.498
-8.537101750D+04-6.487046070D+01 7.047159350D+00-1.843088186D-05 3.992267860D-09
-4.500687950D-13 2.055867395D-17                1.821566655D+04-3.162186125D+00
BrOBr           Hform,Cons: JPCRD 1996 v25 n4 p1069.
 2 j 3/96 BR  2.00O   1.00    0.00    0.00    0.00 0  175.8074000     107639.006
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12399.058
 6.405068910D+04-1.062722566D+03 9.907866290D+00-4.470492470D-03 3.913701070D-06
-1.805444867D-09 3.366132550D-13                1.642921537D+04-2.350319399D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12399.058
-9.686660250D+04-3.957395270D+01 7.029434380D+00-1.171881908D-05 2.576958549D-09
-2.941186078D-13 1.357198784D-17                1.076942321D+04-5.697779380D+00
C               Hf:CJP v33 1955 p125. NSRDS-NBS 3 sec3 1970.
 3 g 7/97 C   1.00    0.00    0.00    0.00    0.00 0   12.0107000     716680.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6535.895
 6.495031470D+02-9.649010860D-01 2.504675479D+00-1.281448025D-05 1.980133654D-08
-1.606144025D-11 5.314483411D-15                8.545763110D+04 4.747924288D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6535.895
-1.289136472D+05 1.719528572D+02 2.646044387D+00-3.353068950D-04 1.742092740D-07
-2.902817829D-11 1.642182385D-15                8.410597850D+04 4.130047418D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6535.895
 4.432528010D+08-2.886018412D+05 7.737108320D+01-9.715281890D-03 6.649595330D-07
-2.230078776D-11 2.899388702D-16                2.355273444D+06-6.405123160D+02
C+              Spec: NSRDS-NBS 3 sec3 1970.
 3 g 6/98 C   1.00E  -1.00    0.00    0.00    0.00 0   12.0101514    1809444.482
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6649.282
 2.258535929D+03-1.574575687D+00 2.503637730D+00-5.202878370D-06 4.516908390D-09
-2.181431053D-12 4.495047033D-16                2.168951913D+05 4.345699505D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6649.282
 1.255112551D+04-3.411874670D+01 2.543383218D+00-2.805120849D-05 9.751641970D-09
-1.736855394D-12 1.246191931D-16                2.171001786D+05 4.063913515D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6649.282
 5.618135320D+05-6.047058900D+03 5.884541470D+00-7.211894530D-04 6.823484110D-08
-2.599878590D-12 3.633868358D-17                2.581370458D+05-2.280019759D+01
C-              JPCRD v14 n3 1985 p731.
 3 g 3/98 C   1.00E   1.00    0.00    0.00    0.00 0   12.0112486     588314.236
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6218.836
 4.671291530D+00-1.986169369D-03 2.500008638D+00-1.976750928D-08 2.478947477D-11
-1.610664044D-14 4.236506810D-18                7.001218550D+04 4.879570141D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6218.836
 4.253175720D+00 5.778186480D-04 2.499999424D+00 2.836136231D-10-7.327253420D-14
 9.478507810D-18-4.830487320D-22                7.001217170D+04 4.879624211D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6218.836
 1.223289007D+01-5.196185830D-03 2.500001344D+00-1.743497251D-10 1.206609009D-14
-4.252419790D-19 5.992333270D-24                7.001221630D+04 4.879608421D+00
CBr             TPIS, vol 2, part 1,1989,p35,157-59.
 2 g 7/95 C   1.00BR  1.00    0.00    0.00    0.00 0   91.9147000     490430.442
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9616.942
 2.940178810D+03-1.404112760D+02 4.754466830D+00-1.646294430D-04 4.345029500D-08
 5.911991170D-11-2.885857060D-14                5.838404230D+04 7.135468684D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9616.942
-4.742652470D+04 5.693118560D+01 4.430118260D+00 9.146508350D-05-6.421129390D-09
 1.437115590D-12-2.606553700D-17                5.719206140D+04 2.907087178D+00
CBr2            TPIS, vol 2, part 1,1991,p39,159-60.
 2 tpis91 C   1.00BR  2.00    0.00    0.00    0.00 0  171.8187000     336623.319
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12196.819
 7.248328410D+04-1.128281265D+03 9.822424480D+00-3.873119170D-03 2.905428646D-06
-1.061887586D-09 1.299148840D-13                4.437781040D+04-2.361188275D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12196.819
-7.441409960D+05 4.215362810D+02 8.796806540D+00-2.726568175D-03 1.336440415D-06
-2.304857484D-10 1.337495860D-14                3.364622190D+04-1.599571545D+01
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CBr3            TPIS, vol 2, part 1,1991,p43,160.
 2 tpis91 C   1.00BR  3.00    0.00    0.00    0.00 0  251.7227000     235000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15582.454
 8.563680670D+04-1.275784656D+03 1.117199833D+01 2.341468231D-03-6.540348360D-06
 5.736478880D-09-1.777748687D-12                3.243226030D+04-2.766524971D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15582.454
-1.925122669D+05-1.327913708D+02 1.009850242D+01-3.917304120D-05 8.612855260D-09
-9.834609870D-13 4.541929600D-17                2.541822955D+04-1.867168433D+01
CBr4            Kudchadker JPCRD v4 n2 1975 p457.
 2 x10/95 C   1.00BR  4.00    0.00    0.00    0.00 0  331.6267000      79500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20373.314
 1.023041073D+05-1.735532220D+03 1.651274909D+01-3.146322486D-03 2.902255614D-07
 1.362374533D-09-6.437335190D-13                1.500470556D+04-5.536243072D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20373.314
-2.061232831D+05-1.044581090D+02 1.307731864D+01-3.066540633D-05 6.723693310D-09
-7.657155210D-13 3.527311030D-17                5.613351190D+03-3.283492572D+01
CCL             TPIS v2 1991. TRC w7270 12/93.
 2 g11/95 C   1.00CL  1.00    0.00    0.00    0.00 0   47.4634000     502100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9394.950
 1.499028985D+04 1.536122028D+01 2.169163834D+00 7.639045640D-03-1.095422627D-05
 7.660858180D-09-2.107668045D-12                5.944752870D+04 1.292263706D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9394.950
-1.695776738D+05 2.200998183D+02 4.200646190D+00 2.328865579D-04-5.365407850D-08
 7.394233880D-12-2.701975375D-16                5.737863620D+04 2.982286879D+00
CCLBr3          TPIS, vol 2, part 1,1991,p94,171.
 2 tpis91 C   1.00CL  1.00BR  3.00    0.00    0.00 0  287.1754000      65000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19568.242
 1.021557592D+05-1.746224860D+03 1.598183983D+01-1.350083121D-03-2.331379435D-06
 3.202885370D-09-1.150729946D-12                1.341940838D+04-5.284903834D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19568.242
-2.282425521D+05-1.278565684D+02 1.309496143D+01-3.782071540D-05 8.331466390D-09
-9.536078550D-13 4.416494600D-17                3.931366430D+03-3.315588474D+01
CCL2            Hf: TRC w7270 12/93. Cons: Misc refs.
 2 g11/95 C   1.00CL  2.00    0.00    0.00    0.00 0   82.9161000     230000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11424.840
 7.461868090D+04-1.027439631D+03 8.010683610D+00 1.703904793D-03-5.047928080D-06
 4.490511400D-09-1.401280705D-12                3.133895996D+04-1.713066208D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11424.840
 1.952527106D+06-7.197819040D+03 1.642671556D+01-6.034435960D-03 1.902519708D-06
-2.592635729D-10 1.282627959D-14                6.988128420D+04-7.500512796D+01
CCL2Br2         TPIS, vol 2, part 1,1991,p98,170-71.
 2 tpis91 C   1.00CL  2.00BR  2.00    0.00    0.00 0  242.7241000      10000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18691.912
 1.018481270D+05-1.740837469D+03 1.521332294D+01 1.128301863D-03-5.875253810D-06
 5.659599550D-09-1.821441324D-12                6.918488030D+03-5.015349200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18691.912
-2.554027577D+05-1.596174508D+02 1.311842248D+01-4.708270280D-05 1.034639123D-08
-1.180574146D-12 5.447689450D-17               -2.589821899D+03-3.461570050D+01
CCL3            TRC 7270 12/93.
 2 x12/93 C   1.00CL  3.00    0.00    0.00    0.00 0  118.3688000      71100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14400.000
 3.414472020D+04-5.547970300D+02 6.845544710D+00 1.242006403D-02-2.036896744D-05
 1.554979891D-08-4.568939810D-12                9.385201480D+03-7.143619254D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14400.000
 2.405028603D+06-8.014855230D+03 1.881204694D+01-5.121309770D-03 1.467000939D-06
-2.016844180D-10 1.062101050D-14                5.583582900D+04-8.535091060D+01
CCL3Br          TPIS, vol 2, part 1,1991,p94,169-70.
 2 tpis91 C   1.00CL  3.00BR  1.00    0.00    0.00 0  198.2728000     -43000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17984.549
 1.049633736D+05-1.793782179D+03 1.489227432D+01 2.397706670D-03-7.790351710D-06
 7.017080730D-09-2.196183079D-12                9.099093500D+02-5.058216164D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17984.549
-2.770914947D+05-1.844184955D+02 1.313714532D+01-5.464709330D-05 1.203130809D-08
-1.374919272D-12 6.352124990D-17               -8.893359870D+03-3.669823794D+01
CCL4            TPIS 1991 v2 pt1 p111; pt2 p84.
 2 tpis91 C   1.00CL  4.00    0.00    0.00    0.00 0  153.8215000     -95600.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17158.512
 1.093385626D+05-1.861731846D+03 1.449632467D+01 3.949485160D-03-1.010805379D-05
 8.645514170D-09-2.642368852D-12 0.000000000D+00-4.948006230D+03-5.180285920D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17158.512
-3.043078255D+05-2.168170491D+02 1.316132386D+01-6.431124890D-05 1.416482497D-08
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-1.619343320D-12 7.483974350D-17 0.000000000D+00-1.512320070D+04-3.996845470D+01
CF              Cons:TPIS,v2,pt1,1989,p35,74. Hf298:TRC w6950,6/88.
 2 g11/95 C   1.00F   1.00    0.00    0.00    0.00 0   31.0091032     242300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9082.053
-4.856590870D+04 8.370668450D+02-1.586053801D+00 1.373299258D-02-1.545437202D-05
 8.898794940D-09-2.083197681D-12                2.419209495D+04 3.371104747D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9082.053
-7.303011730D+04-3.104325519D+02 4.687559650D+00-1.753886181D-05 1.179982950D-08
-1.882833157D-12 1.898119622D-16                2.934902936D+04-2.321779244D+00
CF+             IP and cons: Janaf 12/70
 2 g12/95 C   1.00F   1.00E  -1.00    0.00    0.00 0   31.0085546    1136742.499
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8697.499
-5.975260530D+04 9.276934970D+02-1.866622253D+00 1.384351988D-02-1.513444717D-05
 8.518669310D-09-1.959609178D-12                1.312909185D+05 3.412034117D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8697.499
-8.052380680D+04-3.390680720D+02 4.708419500D+00-3.965717410D-05 2.498748736D-08
-5.237895180D-12 5.314587990D-16                1.370729768D+05-3.920858395D+00
CFBr3           TPIS, vol 2, part 1,1991,p94,166-67.
 2 tpis91 C   1.00F   1.00BR  3.00    0.00    0.00 0  270.7211032    -120000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18243.104
 5.150232570D+04-9.366189820D+02 1.044337268D+01 1.205159881D-02-1.875982024D-05
 1.344258879D-08-3.729863060D-12               -1.243179334D+04-2.364374249D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18243.104
-2.729019621D+05-3.328591750D+02 1.324828118D+01-9.930822180D-05 2.194934877D-08
-2.517564069D-12 1.167020238D-16               -1.730158683D+04-3.626857692D+01
CFCL            TPIS, vol 2, part 1,1991,p39,135-36.
 2 tpis91 C   1.00F   1.00CL  1.00    0.00    0.00 0   66.4618032     25872.113
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10928.721
 1.794757102D+04-1.290180589D+02 2.793459935D+00 1.323564110D-02-1.816297454D-05
 1.213711709D-08-3.214302850D-12                2.623819555D+03 1.166722356D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10928.721
 1.945366777D+06-7.156814800D+03 1.583935195D+01-5.352460090D-03 1.601624273D-06
-2.091786920D-10 9.980836490D-15                4.519921500D+04-7.249953024D+01
CFCLBr2         TPIS, vol 2, part 1,1991,p174-76.
 2 tpis91 C   1.00F   1.00CL  1.00BR  2.00    0.00 0  226.2698032    -175000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17498.023
 5.898428730D+04-1.050657500D+03 1.039314795D+01 1.273794404D-02-1.999260614D-05
 1.438332085D-08-4.000523490D-12               -1.837826616D+04-2.417289968D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17498.023
-2.961695804D+05-3.529024100D+02 1.326323916D+01-1.052749599D-04 2.326118794D-08
-2.666945081D-12 1.235664461D-16               -2.387741139D+04-3.684815638D+01
CFCL2           TPIS, vol 2, part 1,1991,p43,138-39.
 2 tpis91 C   1.00F   1.00CL  2.00    0.00    0.00 0  101.9145032    -105000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13216.954
 2.611533165D+04-3.353754810D+02 4.094775350D+00 1.960217372D-02-2.762737215D-05
 1.880098318D-08-5.047341560D-12               -1.251289778D+04 6.870297529D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13216.954
-2.653089592D+05-4.469903770D+02 1.033337979D+01-1.333901752D-04 2.949592360D-08
-3.384792650D-12 1.569756192D-16               -1.393149991D+04-2.556840439D+01
CFCL2Br         TPIS, vol 2, part 1,1991,p174-75.
 2 tpis91 C   1.00F   1.00CL  2.00BR  1.00    0.00 0  181.8185032    -235000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16730.573
 6.528885750D+04-1.135086759D+03 1.009447171D+01 1.401593294D-02-2.192007992D-05
 1.573622679D-08-4.369970510D-12               -2.504559920D+04-2.450647770D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16730.573
-3.216610680D+05-3.881104830D+02 1.328959746D+01-1.158441537D-04 2.560085910D-08
-2.935547463D-12 1.360237525D-16               -3.097617329D+04-3.871132565D+01
CFCL3           Hf:TRC 7350 6/89. Cons: JPCRD v5 n3 1976 p571.
 2 g10/95 C   1.00F   1.00CL  3.00    0.00    0.00 0  137.3672032    -283700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16080.460
 7.239316600D+04-1.228338402D+03 9.909048890D+00 1.495111116D-02-2.335887731D-05
 1.674757793D-08-4.645208420D-12               -3.032313023D+04-2.644729343D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16080.460
-3.442470690D+05-4.217479500D+02 1.331496258D+01-1.260987797D-04 2.789044161D-08
-3.200596940D-12 1.484096665D-16               -3.671577460D+04-4.157016165D+01
CF2             TRC tuvw6950 6/88.
 2 x 6/88 C   1.00F   2.00    0.00    0.00    0.00 0   50.0075064    -186600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10347.000
-4.284695490D+04 9.422413470D+02-3.838473780D+00 2.847875843D-02-3.618556780D-05
 2.307503213D-08-5.914984890D-12               -2.779937588D+04 4.667598260D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10347.000
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-1.985921862D+06 4.474861080D+03 2.053677908D+00 2.542120168D-03-6.466365360D-07
 7.988225820D-11-3.824522580D-15              -5.434851100D+04 2.288995544D+01
CF2+            IP and cons: Janaf 12/70
 2 g12/95 C   1.00F   2.00E  -1.00    0.00    0.00 0   50.0069578     948480.586
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10352.586
-1.283891178D+03 3.840997350D+02-6.091410750D-01 1.894628635D-02-2.220414306D-05
 1.304882416D-08-3.098609894D-12               1.113939525D+05 2.966035948D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10352.586
 4.014595010D+05-2.428629279D+03 9.472574310D+00-1.266711829D-03 3.203308490D-07
-3.431890470D-11 1.327705535D-15               1.263937635D+05-3.005619598D+01
CF2Br2          TPIS, vol 2, part 1,1991,p98,166.
 2 tpis91 C   1.00F   2.00BR  2.00    0.00    0.00 0  209.8155064    -380000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16279.997
 1.260855554D+04-2.814955512D+02 5.097617420D+00 2.502658682D-02-3.439003900D-05
 2.297717921D-08-6.080431780D-12              -4.642800810D+04 3.096486347D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16279.997
-3.328107240D+05-6.183053530D+02 1.346155155D+01-1.848320799D-04 4.090049080D-08
-4.696059110D-12 2.178674143D-16              -4.715269330D+04-4.105263139D+01
CF2CL           TPIS, vol 2, part 1,1991,p43,136-37.
 2 tpis91 C   1.00F   2.00CL  1.00    0.00    0.00 0   85.4602064    -275000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12432.273
 8.914194930D+03-1.768378144D+01 1.606995743D+00 2.473630328D-02-3.270742130D-05
 2.126352512D-08-5.509828480D-12              -3.427308440D+04 1.929690894D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12432.273
-2.802767108D+05-6.859220450D+02 1.051133006D+01-2.046467037D-04 4.527806960D-08
-5.199139530D-12 2.412622798D-16              -3.308250760D+04-2.874822953D+01
CF2CLBr         TPIS, vol 2, part 1,1991,p173-74.
 2 tpis91 C   1.00F   2.00CL  1.00BR  1.00    0.00 0  165.3642064    -435000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15528.243
 2.696919535D+04-4.679154430D+02 5.244994810D+00 2.530067254D-02-3.508358910D-05
 2.354286863D-08-6.245950200D-12              -5.198367380D+04 8.522604855D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15528.243
-3.593574950D+05-6.536987130D+02 1.348804664D+01-1.954573318D-04 4.325315000D-08
-4.966206660D-12 2.303958492D-16              -5.365286690D+04-4.224722904D+01
CF2CL2          Hf:TRC 7350 6/89. Cons: JPCRD v5 n3 1976 p571.
 2 g10/95 C   1.00F   2.00CL  2.00    0.00    0.00 0  120.9129064    -490800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14873.998
 3.844509960D+04-6.132645270D+02 5.256201720D+00 2.576477732D-02-3.588861610D-05
 2.411672631D-08-6.400485150D-12              -5.784612020D+04-1.893431345D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14873.998
-3.828465550D+05-6.960315140D+02 1.351991590D+01-2.083222216D-04 4.612086630D-08
-5.297664520D-12 2.458667174D-16              -6.020072810D+04-4.482433645D+01
CF3             Cons:TPIS,v2,pt1,1991,p43,77. Hf298:TRC w6950 6/88.
 2 g11/95 C   1.00F   3.00    0.00    0.00    0.00 0   69.0059096    -467400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11479.084
-2.895093138D+04 7.082591040D+02-3.498744960D+00 3.600527790D-02-4.518456380D-05
 2.830460969D-08-7.124280160D-12              -6.055799540D+04 4.500436386D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11479.084
-3.009925372D+05-1.045774154D+03 1.077830669D+01-3.112228054D-04 6.882330840D-08
-7.900181810D-12 3.665106310D-16              -5.426367000D+04-3.416192034D+01
CF3+            IP and cons: Janaf 12/71
 2 g12/95 C   1.00F   3.00E  -1.00    0.00    0.00 0   69.0053610     423632.578
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11543.578
 2.192882878D+04 1.715078816D+01 5.187199500D-01 2.442834350D-02-2.866389833D-05
 1.675377163D-08-3.951053180D-12               4.990840940D+04 2.168928467D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11543.578
-2.373522001D+05-1.280239400D+03 1.094410483D+01-3.751093500D-04 8.256758650D-08
-9.445297810D-12 4.370448090D-16               5.440587470D+04-3.672366714D+01
CF3Br           TPIS, vol 2, part 1,1991,p94,165-66.
 2 tpis91 C   1.00F   3.00BR  1.00    0.00    0.00 0  148.9099096    -648800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14444.028
-5.436765740D+03 1.243244917D+02 9.233860680D-01 3.480995660D-02-4.549581320D-05
 2.932794817D-08-7.547895280D-12              -8.023378790D+04 2.232890591D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14444.028
-3.834194210D+05-9.718927810D+02 1.372477460D+01-2.901840826D-04 6.422676280D-08
-7.377417450D-12 3.424453640D-16              -7.765318430D+04-4.717365875D+01
CF3CL           Hf:TRC 7350 6/89. Cons: JPCRD v5 n3 1976 p571.
 2 g10/95 C   1.00F   3.00CL  1.00    0.00    0.00 0  104.4586096    -704200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13770.726
 1.729454028D+04-1.651867787D+02 1.544194464D+00 3.395737010D-02-4.474835440D-05
 2.894934417D-08-7.464316290D-12              -8.532417310D+04 1.668147013D+01
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13770.726
-4.091360540D+05-1.013156215D+03 1.375548856D+01-3.024564474D-04 6.693716700D-08
-7.688035910D-12 3.568292530D-16               -8.416652620D+04-4.909398931D+01
CF4             TPIS,v2,pt1,1991,p44,79.  TRC w-6880, 12/89.
 2 g10/95 C   1.00F   4.00    0.00    0.00    0.00 0   88.0043128    -933500.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12730.313
 9.815349640D+03 1.163660743D+02-1.288527575D+00 3.959623880D-02-4.996336050D-05
 3.125414298D-08-7.841942110D-12               -1.138960831D+05 2.938759613D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12730.313
-4.164183790D+05-1.414899259D+03 1.405138627D+01-4.199964070D-04 9.281677640D-08
-1.064996410D-11 4.939554390D-16               -1.095141882D+05-5.487202173D+01
CH              Props & Hf0: TPIS,v2,pt2,1979.
 3 tpis79 C   1.00H   1.00    0.00    0.00    0.00 0   13.0186400     597338.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8625.000
 2.220564134D+04-3.405371750D+02 5.531386410D+00-5.794896390D-03 7.969461730D-06
-4.465859890D-09 9.596228840D-13               7.240390520D+04-9.107636130D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8625.000
 2.060733772D+06-5.396129640D+03 7.856187940D+00-7.965757980D-04 1.764273769D-07
-1.976345857D-11 5.030286680D-16               1.062192450D+05-3.154718017D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8625.000
-8.068267550D+08 4.575393220D+05-9.843851280D+01 1.235228588D-02-8.485502230D-07
 3.040372611D-11-4.400260280D-16               -3.595809570D+06 8.953364358D+02
CH+             Props & IP: TPIS,v2,pt2,1991,p41.
 3 tpis91 C   1.00H   1.00E  -1.00    0.00    0.00 0   13.0180914    1630532.000
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8628.000
 3.019567000D+04-4.618081420D+02 6.225564340D+00-7.775613670D-03 1.094475740D-05
-6.675403810D-09 1.565212580D-12               1.972444860D+05-1.431501373D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8628.000
-7.102008540D+06 1.828332720D+04-1.312675460D+01 6.191642170D-03-2.909384530D-07
-1.134230140D-10 1.105948890D-14               7.540973240D+04 1.243969059D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8628.000
-3.160033590D+08 1.436682680D+05-1.108431220D+01 1.562278950D-04 4.928432400D-08
-2.896835540D-12 4.982193740D-17               -1.013663450D+06 1.489335649D+02
CHBr3           Kudchadker JPCRD v4 n2 1975 p457.
 2 x10/95 C   1.00H   1.00BR  3.00    0.00    0.00 0  252.7306400      16700.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15906.601
 4.346130430D+04-4.998999300D+02 5.619870630D+00 2.079443509D-02-2.921478846D-05
 2.067048032D-08-5.781530890D-12               2.622714607D+03 1.249857522D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15906.601
 6.274122180D+05-3.378679150D+03 1.487849130D+01-5.932561680D-04 1.082376390D-07
-1.060966928D-11 4.319033220D-16               1.876733073D+04-5.311884786D+01
CHCL            TPIS v2 1991.TRC w7270 12/93.Jacox JPCRD v19 1990 p1403
 2 gll/95 C   1.00H   1.00CL  1.00    0.00    0.00 0   48.4713400     297100.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10154.502
-1.351685347D+04 5.045204380D+02-1.238174663D+00 2.118629432D-02-3.140702866D-05
 2.447650281D-08-7.264460900D-12               3.247285960D+04 3.179808964D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10154.502
 9.452674480D+06-2.773825775D+04 3.305317660D+01-1.049076690D-02 2.188430036D-06
-2.308780201D-10 9.758053260D-15               2.121039456D+05-2.072912849D+02
CHCLBr2         TPIS, vol 2, part 1,1991,p149,173.
 2 tpis91 C   1.00H   1.00CL  1.00BR  2.00    0.00 0  208.2793400      10000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15291.236
 3.815664790D+04-4.084606340D+02 4.639498200D+00 2.325916256D-02-3.222874940D-05
 2.254584339D-08-6.256248400D-12               1.484013090D+03 6.173832488D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15291.236
 6.043539620D+05-3.438418330D+03 1.494180471D+01-6.229305810D-04 1.153948921D-07
-1.147577581D-11 4.734917430D-16               1.822576072D+04-5.407389182D+01
CHCL2           TRC 7270 12/93.
 2 x12/93 C   1.00H   1.00CL  2.00    0.00    0.00 0   83.9240400      95800.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12800.000
 5.638555970D+04-6.562455130D+02 6.068817860D+00 9.744123060D-03-1.275310200D-05
 8.552387240D-09-2.231582854D-12               1.330447784D+04-4.533556004D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12800.000
 8.849403010D+05-3.526971980D+03 1.186372370D+01-5.002386540D-04 6.133886860D-08
-1.885467132D-12-1.234204469D-16               3.071137949D+04-4.088909582D+01
CHCL2Br         TPIS, vol 2, part 1,1991,p149,172-73.
 2 tpis91 C   1.00H   1.00CL  2.00BR  1.00    0.00 0  163.8280400     -45000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14729.895
 3.293936130D+04-3.275193220D+02 3.773186760D+00 2.536475536D-02-3.472673740D-05
 2.404666102D-08-6.621713290D-12               -5.425618610D+03 9.433686366D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14729.895
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 5.924759410D+05-3.509428180D+03 1.499343143D+01-6.432667140D-04 1.198461557D-07
-1.198298706D-11 4.968927200D-16              1.197222316D+04-5.602643280D+01
CHCL3           TPIS, vol 2, part 1,1991,p94,127-29, PANDK.
 2 g 6/95 C   1.00H   1.00CL  3.00    0.00    0.00 0  119.3767400    -102700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14305.493
 3.395393040D+04-3.047507147D+02 2.923709560D+00 2.830540186D-02-3.712418980D-05
 2.551366712D-08-6.987677410D-12              -1.235059314D+04 1.115533378D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14305.493
 6.134218840D+05-3.714555120D+03 1.510718257D+01 2.365784734D-04 1.296237935D-07
-1.266225803D-11 5.252017700D-16              6.199911820D+03-5.992154424D+01
CHF             TRC uvw6950 6/88.
 2 x 6/88 C   1.00H   1.00F   1.00    0.00    0.00 0   32.0170432     108800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9983.000
-4.538708070D+04 8.734685250D+02-1.973724720D+00 1.717399978D-02-1.929626737D-05
 1.277241064D-08-3.395878240D-12              7.928636920D+03 3.640755969D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9983.000
 7.670328620D+06-2.286073931D+04 2.768821442D+01-7.752178170D-03 1.514767538D-06
-1.586869435D-10 6.915350650D-15              1.580108059D+05-1.703858790D+02
CHFBr2          TPIS, vol 2, part 1,1991,p149,168-69.
 2 tpis91 C   1.00H   1.00F   1.00BR  2.00    0.00 0  191.8250432    -175000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14359.556
-1.820496548D+04 4.362668940D+02-3.736144710D-01 3.388694370D-02-4.371391680D-05
 2.889640212D-08-7.684132790D-12              -2.465631752D+04 3.320606231D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14359.556
 5.935682480D+05-3.742650290D+03 1.517184840D+01-7.158171030D-04 1.360702380D-07
-1.386031011D-11 5.845169590D-16              -2.347729721D+03-5.765787939D+01
CHFCL           TPIS, vol 2, part 1,1991,p43,147.
 2 tpis91 C   1.00H   1.00F   1.00CL  1.00    0.00 0   67.4697432     -83144.704
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11145.955
-7.113033040D+04 1.377875844D+03-6.484631940D+00 3.890975950D-02-4.800739870D-05
 3.073303617D-08-7.982865720D-12              -1.751795274D+04 6.373902956D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11145.955
 6.621501210D+05-3.808823140D+03 1.223860673D+01-7.466143100D-04 1.434485105D-07
-1.475026402D-11 6.271787140D-16              1.018868887D+04-4.658224084D+01
CHFCLBr         TPIS, vol 2, part 1,1991,p149,176.
 2 tpis91 C   1.00H   1.00F   1.00CL  1.00BR  1.00 0  147.3737432    -230000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13787.186
-1.959516997D+04 4.902099240D+02-1.259605377D+00 3.617759590D-02-4.654315050D-05
 3.065289129D-08-8.124036330D-12              -3.139918926D+04 3.710561029D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13787.186
 5.798945860D+05-3.823011260D+03 1.522774213D+01-7.372079790D-04 1.406599886D-07
-1.437574370D-11 6.080338360D-16              -8.554350940D+03-5.903426791D+01
CHFCL2          Hf:TRC 7350 6/89. Cons: JPCRD v5 n3 1976 p571.
 2 g10/95 C   1.00H   1.00F   1.00CL  2.00    0.00 0  102.9224432    -284900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13285.927
-1.788703489D+04 4.974836600D+02-1.871479110D+00 3.783471130D-02-4.860890010D-05
 3.193804160D-08-8.446131160D-12              -3.791317790D+04 3.810590195D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13285.927
 5.656971960D+05-3.891992710D+03 1.527881230D+01-7.575777970D-04 1.451605718D-07
-1.489241700D-11 6.320194000D-16              -1.481478470D+04-6.170725235D+01
CHF2            TRC uvw6950 6/88.
 2 x 6/88 C   1.00H   1.00F   2.00    0.00    0.00 0   51.0154464    -238900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10920.000
-1.469690135D+05 2.553397322D+03-1.302627636D+01 5.438128480D-02-6.713418820D-05
 4.287651750D-08-1.110824219D-11              -4.179372170D+04 9.939928516D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10920.000
 5.526811910D+05-3.696010420D+03 1.208610698D+01-6.498594170D-04 1.120847764D-07
-9.814166670D-12 3.349202240D-16              -9.437060220D+03-4.704418874D+01
CHF2Br          TPIS, vol 2, part 1,1991,p149,168.
 2 tpis91 C   1.00H   1.00F   2.00BR  1.00    0.00 0  130.9194464    -422000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13169.504
-7.714715990D+04 1.422575306D+03-6.684578460D+00 4.738443270D-02-5.830671530D-05
 3.695783430D-08-9.495672470D-12              -5.878515710D+04 6.608740382D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13169.504
 5.767321960D+05-4.177610910D+03 1.550139673D+01-8.489597160D-04 1.657036632D-07
-1.727655652D-11 7.434843210D-16              -2.966215259D+04-6.349301408D+01
CHF2CL          Hf:TRC 7350 6/89. Cons: JPCRD v5 n3 1976 p571.
 2 g10/95 C   1.00H   1.00F   2.00CL  1.00    0.00 0   86.4681464    -482800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12362.102
-7.153574920D+04 1.355123563D+03-7.123880370D+00 4.854763810D-02-5.955274850D-05
 3.758361960D-08-9.614866150D-12              -6.560543580D+04 6.637489699D+01
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12362.102
 5.622668410D+05-4.293100440D+03 1.557620973D+01-8.762857570D-04 1.713910807D-07
-1.790263798D-11 7.716735770D-16              -3.637400570D+04-6.607130761D+01
CHF3            TPIS,v2,pt1,1991,p94,97,NRRAO1. TRC w-6880, 12/89.
 2 g10/95 C   1.00H   1.00F   3.00    0.00    0.00 0   70.0138496    -693300.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11566.886
-1.095134981D+05 2.042274994D+03-1.166211829D+01 5.785798380D-02-6.857112170D-05
 4.212094800D-08-1.053188135D-11              -9.395470900D+04 8.935915074D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11566.886
 5.685939530D+05-4.728569680D+03 1.586751918D+01-7.383628500D-04 1.971201615D-07
-2.062614684D-11 8.973291810D-16              -5.923063710D+04-7.161441636D+01
CH2             Hf298: TRC tables.  Cons: JPCRD v17,1988,p279.
 2 g11/89 C   1.00H   2.00    0.00    0.00    0.00 0   14.0265800     388800.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10027.422
 3.525914180D+04-3.367654360D+02 4.508936910D+00 2.521066030D-03-5.311510870D-06
 6.654213080D-09-2.610072960D-12               4.737725500D+04-3.807404284D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10027.422
 2.510415940D+06-7.953932390D+03 1.238829570D+01-1.775909680D-03 3.217400290D-07
-3.068863440D-11 1.204900600D-15               9.601028560D+04-6.155984406D+01
CH2Br2          Kudchadker JPCRD v4 n2 1975 p457.
 2 x10/95 C   1.00H   2.00BR  2.00    0.00    0.00 0  173.8345800    -14800.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12614.407
 4.793752150D+03 3.614336800D+02-1.819837582D+00 3.477110360D-02-4.498628610D-05
 3.068678987D-08-8.434994370D-12              -4.485337420D+03 3.827261792D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12614.407
 1.528243720D+06-6.673302110D+03 1.670201067D+01-1.166284445D-03 2.122443611D-07
-2.075202879D-11 8.427112710D-16               3.600273290D+04-7.447977708D+01
CH2CL           TPIS v2 1991.TRC w7270 12/93. JPCRD v19 1990 p1387
 2 g 2/96 C   1.00H   2.00CL  1.00    0.00    0.00 0   49.4792800     119200.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10979.920
-3.188772250D+04 6.333417390D+02-1.164198028D+00 2.160620041D-02-2.545507624D-05
 1.693918152D-08-4.660158650D-12               1.020130219D+04 3.230909172D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10979.920
 1.662402020D+06-6.441034710D+03 1.359745277D+01-1.140500096D-03 2.087681942D-07
-2.052270373D-11 8.375506900D-16               5.212846460D+04-6.148524708D+01
CH2CLBr         TPIS, vol 2, part 1,1991,p98,171-72.
 2 tpis91 C   1.00H   2.00CL  1.00BR  1.00    0.00 0  129.3832800    -45000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12190.747
-1.308560298D+04 6.456728250D+02-3.577829250D+00 3.833819870D-02-4.864447070D-05
 3.261767450D-08-8.853305960D-12              -9.402688990D+03 4.749072774D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12190.747
 1.525025678D+06-6.823360110D+03 1.682772117D+01-1.219753973D-03 2.245029358D-07
-2.219175161D-11 9.105447920D-16               3.320256530D+04-7.637593106D+01
CH2CL2          TPIS, vol 2, part 1,1991,p98,125-27.
 2 tpis91 C   1.00H   2.00CL  2.00    0.00    0.00 0   84.9319800    -95000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11854.077
-2.509741052D+04 8.687522530D+02-5.094588190D+00 4.150027530D-02-5.199739730D-05
 3.445921160D-08-9.270228940D-12              -1.638971913D+04 5.396843710D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11854.077
 1.529283055D+06-6.976970440D+03 1.694156830D+01-1.265063076D-03 2.344786301D-07
-2.333245612D-11 9.632891700D-16               2.806327866D+04-7.949468800D+01
CH2F            TRC uvw6950 6/88.
 2 x 6/88 C   1.00H   2.00F   1.00    0.00    0.00 0   33.0249832    -31800.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11129.000
-8.569713230D+04 1.392226838D+03-4.382053100D+00 2.645917089D-02-2.848145873D-05
 1.732706186D-08-4.442061910D-12              -1.169444629D+04 5.049496755D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11129.000
-3.593751570D+08 9.211304900D+05-8.874297700D+02 4.271265490D-01-1.062480192D-04
 1.323316726D-08-6.500709300D-13              -6.015409460D+06 6.529098563D+03
CH2FBr          TPIS, vol 2, part 1,1991,p98,167-68.
 2 tpis91 C   1.00H   2.00F   1.00BR  1.00    0.00 0  112.9289832    -215000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11622.585
-9.256139710D+04 1.811990123D+03-9.698369970D+00 5.035854820D-02-6.070281320D-05
 3.878257000D-08-1.012617780D-11              -3.537511670D+04 8.140408563D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11622.585
 1.539996347D+06-7.231619950D+03 1.714575038D+01-1.350236508D-03 2.538184169D-07
-2.559220117D-11 1.069450769D-15               1.509647220D+04-8.062114847D+01
CH2FCl          Hf:TRC 7350 6/89. Cons: JPCRD v5 n3 1976 p571.
 2 g10/95 C   1.00H   2.00F   1.00CL  1.00    0.00 0   68.4776832    -265700.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11252.779
-1.074853941D+05 2.089158857D+03-1.161911339D+01 5.463012120D-02-6.551723550D-05
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 4.157073700D-08-1.078607505D-11              -4.268199300D+04 9.068454746D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11252.779
 1.533648782D+06-7.369660710D+03 1.725145396D+01-1.393149144D-03 2.633907453D-07
-2.669680565D-11 1.120868106D-15              9.754463640D+03-8.308254954D+01
CH2F2           TPIS,v2,pt1,1991,p96. TRC w-6880, 12/89.
 2 g10/95 C   1.00H   2.00F   2.00    0.00    0.00 0   52.0233864    -452300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10693.327
-1.819922125D+05 3.174433370D+03-1.714259234D+01 6.411358170D-02-7.313595650D-05
 4.426384980D-08-1.103877045D-11              -7.027061700D+04 1.207333210D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10693.327
 1.546546355D+06-7.876703830D+03 1.768750495D+01-1.581187710D-03 3.068594074D-07
-3.182938480D-11 1.363564482D-15              -9.801285300D+03-8.907278100D+01
CH3             Hf298: TRC Apr30,1989. Cons: JPCRD V17,1988,p3526.
 2 g11/89 C   1.00H   3.00    0.00    0.00    0.00 0   15.0345200     146900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10366.340
-2.877286110D+04 5.095056070D+02 1.990730560D-01 1.363965160D-02-1.434558920D-05
 1.013967380D-08-3.028438890D-12               1.411098730D+04 2.023388634D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10366.340
 2.760904270D+06-9.336552790D+03 1.487698630D+01-1.439227690D-03 2.443923930D-07
-2.223845790D-11 8.391588490D-16               7.484764790D+04-7.919489326D+01
CH3Br           Kudchadker JPCRD v4 n2 1975 p457.
 2 x10/95 C   1.00H   3.00BR  1.00    0.00    0.00 0   94.9385200     -37700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10612.655
-7.115597990D+04 1.524707170D+03-8.230448980D+00 4.239973300D-02-4.946978720D-05
 3.194431700D-08-8.531230550D-12              -1.251273152D+04 7.048135432D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10612.655
 2.524823219D+06-1.011862235D+04 1.865887871D+01-1.797601631D-03 3.298331660D-07
-3.250667310D-11 1.330055934D-15              5.540967860D+04-9.778555538D+01
CH3CL           TPIS, vol 2, part 1,1991,p94,122-24.
 2 tpis91 C   1.00H   3.00CL  1.00    0.00    0.00 0   50.4872200     -81870.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10416.144
-9.841987770D+04 1.983702303D+03-1.084512616D+01 4.777979800D-02-5.515515010D-05
 3.506175200D-08-9.236102840D-12              -1.994690300D+04 8.399658748D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10416.144
 2.522470775D+06-1.030118166D+04 1.882729495D+01-1.872314346D-03 3.473445520D-07
-3.458996030D-11 1.429002463D-15              5.111434230D+04-1.006574120D+02
CH3F            TPIS,v2,pt1,1991,p93. TRC w-6880, Dec.1989.
 2 g10/95 C   1.00H   3.00F   1.00    0.00    0.00 0   34.0329232    -237700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10135.229
-2.029825364D+05 3.447335770D+03-1.768996723D+01 5.945282620D-02-6.469539320D-05
 3.859427790D-08-9.626576520D-12              -4.577928480D+04 1.228383412D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10135.229
 2.561892955D+06-1.086051204D+04 1.929446743D+01-2.070980107D-03 3.929165270D-07
-3.994586640D-11 1.681504828D-15              3.563497160D+04-1.061158311D+02
CH2OH           Hydroxymethylene rad. Multiple refns.
 2 g12/92 C   1.00H   3.00O   1.00    0.00    0.00 0   31.0339200      -8900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11833.908
-8.233171980D+04 1.300536350D+03-4.166378350D+00 3.033934820D-02-3.407934070D-05
 2.178948850D-08-5.794730600D-12              -8.602010100D+03 4.926176910D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11833.908
 2.528592310D+06-9.235951970D+03 1.712908490D+01-1.310755350D-03 2.136469110D-07
-1.871002940D-11 6.849718830D-16              5.418395600D+04-8.674895020D+01
CH3O            Hf298: TPIS 1991. Cons: JPCRD v17 n2,1988,p419.
 2 g10/92 C   1.00H   3.00O   1.00    0.00    0.00 0   31.0339200      13000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10745.287
-2.829626980D+04 6.761963280D+02-2.279165650D+00 2.423344780D-02-2.209351630D-05
 1.230458840D-08-3.104673130D-12              -2.609291450D+03 3.633785760D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10745.287
 2.224626760D+06-9.720565480D+03 1.882482040D+01-1.961522810D-03 3.790769080D-07
-3.964690740D-11 1.792380020D-15              5.842931850D+04-1.004168110D+02
CH4             Cons & Hf298: TPIS v2,pt1,1991.
 2 g 8/88 C   1.00H   4.00    0.00    0.00    0.00 0   16.0424600     -74600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10016.198
-1.766545730D+05 2.785477820D+03-1.201935470D+01 3.914625880D-02-3.611656080D-05
 2.018387940D-08-4.955772150D-12              -2.331011560D+04 8.901075390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10016.198
 3.746265700D+06-1.388851340D+04 2.054029820D+01-1.944196930D-03 4.323871450D-07
-4.061012780D-11 1.643159270D-15              7.565988680D+04-1.222977672D+02
CH3OH           Cons: JPCRD v6 n1,1977,p105. Hf298: TRC w5030,6/30/87.
 2 g 8/88 C   1.00H   4.00O   1.00    0.00    0.00 0   32.0418600    -200940.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11435.277
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-2.416637470D+05 4.032138120D+03-2.046409540D+01 6.903679330D-02-7.598902310D-05
 4.598184380D-08-1.158699450D-11              -4.433256970D+04 1.400138860D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11435.277
 3.411560750D+06-1.345497450D+04 2.261404600D+01-2.141011990D-03 3.729997540D-07
-3.498763320D-11 1.366022140D-15                5.636063860D+04-1.277812260D+02
CI             TPIS, vol 2, part 1,1989,p35,176-77.
 2 g 7/95 C   1.00I   1.00    0.00    0.00    0.00 0  138.9151700     570200.657
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9497.157
 1.035862250D+05-1.705781370D+03 1.283820130D+01-1.814743200D-02 2.116317580D-05
-1.273899660D-08 3.129522290D-12                7.546087800D+04-4.468449868D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9497.157
-2.718172240D+04 2.030028660D+02 4.348515960D+00 1.269726810D-04-1.052998870D-08
 1.567555920D-12-7.177736160D-17                6.599585840D+04 4.651562322D+00
CN             Props:TPIS v2 pt2 1991. Hf:JPC v96 1992 p425.
 3 g 3/96 C   1.00N   1.00    0.00    0.00    0.00 0   26.0174400     438683.448
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8672.000
 3.949101750D+03-1.391573871D+02 4.930776040D+00-6.304594730D-03 1.256821364D-05
-9.878181750D-09 2.843103040D-12                5.228454700D+04-2.763114588D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8672.000
-2.227976079D+06 5.040664450D+03-2.121794479D-01 1.354881217D-03 1.325922767D-07
-6.936934000D-11 5.494891620D-15                1.784542332D+04 3.282515520D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8672.000
-1.794773071D+08 1.054331428D+05-1.729598876D+01 2.194863831D-03-8.508801680D-08
 9.318468300D-13 6.358214080D-18               -7.962476450D+05 1.913112387D+02
CN+            Props & Hf0: TPIS v2,pt2,1991,p203.
 3 tpis91 C   1.00N   1.00E  -1.00    0.00    0.00 0   26.0168914    1800490.876
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8682.000
-8.302801010D+05 8.775572030D+03-2.977403223D+01 4.976826600D-02-1.302196808D-05
-2.058309431D-08 1.126832679D-11                1.705790877D+05 2.039891361D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8682.000
-7.153374510D+06 1.857227457D+04-1.084520530D+01 6.106605260D-03-1.191193565D-06
 1.184833689D-10-4.799776870D-15                9.262041240D+04 1.135326165D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8682.000
-1.812946307D+08 1.128804516D+05-2.287308390D+01 3.484585730D-03-2.209762556D-07
 6.579765390D-12-7.556495860D-17               -6.784208570D+05 2.362633451D+02
CN-            Cons & Hf0: TPIS v2,pts1&2,1991.
 2 g10/92 C   1.00N   1.00E   1.00    0.00    0.00 0   26.0179886      65485.578
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.558
-4.594417730D+04 4.266617720D+02 2.347624400D+00-1.813025170D-04 4.566251290D-06
-4.467934810D-09 1.367138460D-12                4.566971260D+03 1.132722411D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.558
 3.478824580D+05-1.621467950D+03 5.602458700D+00-3.944482450D-04 8.731643390D-08
-9.684711420D-12 4.377563990D-16                1.661227120D+04-1.169938609D+01
CNN            TPIS 1991. JPCRD v17,1988,p314. JCP v67 n2,1977,p664.
 2 g12/89 C   1.00N   2.00    0.00    0.00    0.00 0   40.0241800     633474.702
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10368.306
-1.347069570D+03-1.384815980D+02 4.591760420D+00 4.297020730D-03-4.265777430D-06
 2.940565300D-09-8.910137610D-13                7.544582930D+04 1.609001236D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10368.306
 6.085327250D+05-2.582435060D+03 8.694926160D+00-1.826896780D-04-1.360350150D-08
 8.576679930D-12-5.807255010D-16                9.021215030D+04-2.721343348D+01
CO             Props & Hf298: TPIS vo2,pt2,1979,p29.
 3 tpis79 C   1.00O   1.00    0.00    0.00    0.00 0   28.0101000    -110530.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.000
 1.489027557D+04-2.922250947D+02 5.724458410D+00-8.176136940D-03 1.456885983D-05
-1.087733246D-08 3.027905485D-12               -1.303069697D+04-7.859179282D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.000
 4.619158560D+05-1.944685748D+03 5.916647090D+00-5.664234070D-04 1.398802571D-07
-1.787664983D-11 9.620850400D-16               -2.465738441D+03-1.387402604D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.000
 8.868552410D+08-7.500285410D+05 2.495444488D+02-3.956302990D-02 3.297732100D-06
-1.318393976D-10 1.998913781D-15                5.701351240D+06-2.060679613D+03
CO+            Props and Hf0: TPIS,v2,pt2,1991,p22.
 3 tpis91 C   1.00O   1.00E  -1.00    0.00    0.00 0   28.0095514    1247790.876
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.000
-2.178739990D+04 1.288818190D+02 3.769022890D+00-3.431713910D-03 8.193879110D-06
-6.463757900D-09 1.803711430D-12                1.482348250D+05 3.990405688D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.000
 2.316816600D+05-1.057632630D+03 4.554202310D+00 4.495469340D-04-2.489477820D-07
 5.267503910D-11-3.289471100D-15                1.555052030D+05-3.873442982D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.000
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-3.035557230D+08 2.393083920D+05-7.034901960D+01 1.139536280D-02-8.315064010D-07
 2.863668140D-11-3.803219840D-16              -1.688590830D+06 6.291893329D+02
COCL            TPIS, vol 2, part 1,1991,p30,118-19.
 2 tpis91 C   1.00O   1.00CL  1.00    0.00    0.00 0   63.4628000    -16000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11550.749
 2.513189017D+04-5.969223670D+02 8.327700470D+00-7.056246430D-03 1.313172555D-05
-1.037079568D-08 3.033734254D-12              -7.052624050D+02-1.580733271D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11550.749
 3.443208570D+05-1.793002700D+03 8.392606860D+00-5.373985570D-04 9.111384780D-08
-3.108433536D-12-2.042072504D-16               6.913562930D+03-1.998812919D+01
COCL2           Carbonic Dichloride.
 2 tpis91 C   1.00O   1.00CL  2.00    0.00    0.00 0   98.9155000    -219500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12878.622
 9.319010400D+04-1.577929126D+03 1.208332035D+01-4.808457290D-03 7.687730900D-06
-5.858340390D-09 1.687653586D-12              -2.054272785D+04-3.834645430D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12878.622
-2.546127725D+04-1.305943380D+03 1.092919845D+01-3.600996590D-04 7.786236790D-08
-8.791135930D-12 4.027875600D-16              -2.219856143D+04-3.233286300D+01
COF             TPIS, vol 2, part 1,1991,p30,87-89.
 2 tpis91 C   1.00O   1.00F   1.00    0.00    0.00 0   47.0085032    -179413.270
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10392.836
 1.215778086D+04-6.593526620D+01 3.021551071D+00 7.487976780D-03-6.166939750D-06
 2.391387152D-09-3.361122200D-13              -2.234565878D+04 1.061586218D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10392.836
 2.084365824D+05-1.775462902D+03 8.320092050D+00-4.815486580D-04 7.389191450D-08
-1.035536242D-12-2.879005298D-16              -1.320349610D+04-2.203392272D+01
COFCL           TPIS, vol 2, part 1,1991,p61,146-47.
 2 tpis91 C   1.00O   1.00F   1.00CL  1.00    0.00 0   82.4612032    -429492.862
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11903.798
 7.262160960D+04-1.019737504D+03 7.290916090D+00 7.420655940D-03-7.902460570D-06
 4.209341150D-09-9.314113080D-13              -4.804386910D+04-1.316926202D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11903.798
-5.320859910D+04-1.580898321D+03 1.112684431D+01-4.372354340D-04 9.462384470D-08
-1.069041024D-11 4.900404730D-16              -4.599738750D+04-3.525794032D+01
COF2            Carbonic Difluoride.
 2 tpis91 C   1.00O   1.00F   2.00    0.00    0.00 0   66.0069064    -640000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11133.929
 5.263416560D+04-4.618640020D+02 2.774136876D+00 1.831924268D-02-2.130161693D-05
 1.266915940D-08-3.101649325D-12              -7.564253380D+04 9.467052465D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11133.929
-4.072852820D+04-1.974036774D+03 1.140366508D+01-5.437255000D-04 1.175269803D-07
-1.326611381D-11 6.077009710D-16              -6.907778080D+04-4.009716354D+01
COHCL           TPIS, vol 2, part 1,1991,p61,134-35.
 2 tpis91 C   1.00O   1.00H   1.00CL  1.00    0.00 0   64.4707400    -164211.876
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11006.282
 6.331749190D+03 8.122023710D+01 1.374559349D+00 1.650994511D-02-1.692951707D-05
 9.684301160D-09-2.374545007D-12              -2.120364581D+04 1.938428054D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11006.282
 8.318835510D+05-4.416843720D+03 1.270658744D+01-9.361307070D-04 1.855313386D-07
-1.958355847D-11 8.511970980D-16               4.330316640D+03-5.145055356D+01
COHF            TPIS, vol 2, part 1,1991,p61,106.
 2 tpis91 C   1.00O   1.00H   1.00F   1.00    0.00 0   48.0164432    -374590.361
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10449.795
-4.585914070D+04 1.048213577D+03-4.776626210D+00 3.080731808D-02-3.415909630D-05
 2.034934410D-08-5.054210110D-12              -5.085989100D+04 5.232276276D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10449.795
 8.578998850D+05-4.791999300D+03 1.293979389D+01-1.018305688D-03 2.021327317D-07
-2.136752030D-11 9.299800180D-16              -1.878907196D+04-5.527480364D+01
COS             TPIS, vol 2, part 1,1991,p28,211-12,NRRAO1.
 2 g 6/95 C   1.00O   1.00S   1.00    0.00    0.00 0   60.0761000    -141700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9941.597
 8.547944370D+04-1.319473564D+03 9.735300420D+00-6.870939300D-03 1.082346243D-05
-7.705702740D-09 2.078600560D-12              -1.191653394D+04-2.992011353D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9941.597
 1.958696362D+05-1.756061149D+03 8.710321830D+00-4.138878210D-04 1.015099651D-07
-1.159420921D-11 5.690088200D-16              -8.927787370D+03-2.636247495D+01
CO2             Props & Hf298: TPIS v2,pt1,1991,p27.
 3 g 7/88 C   1.00O   2.00    0.00    0.00    0.00 0   44.0095000    -393510.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9365.469
 4.943783640D+04-6.264292080D+02 5.301813360D+00 2.503600571D-03-2.124700099D-07
-7.691486800D-10 2.849979913D-13              -4.528189860D+04-7.048790100D+00
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9365.469
 1.176969434D+05-1.788801467D+03 8.291543530D+00-9.224778310D-05 4.869635410D-09
-1.892063841D-12 6.330675090D-16              -3.908345010D+04-2.652683962D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9365.469
-1.544406228D+09 1.016836139D+06-2.561377096D+02 3.369363930D-02-2.181157911D-06
 6.991324850D-11-8.842212140D-16              -8.043128500D+06 2.254153243D+03
CO2+            Cons&Hf0: TPIS,v2,pt1,1991,p30.
 3 g10/92 C   1.00O   2.00E  -1.00    0.00    0.00 0   44.0089514     944684.912
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10566.089
-7.383068120D+04 1.086218050D+03-2.771150320D+00 2.318474130D-02-2.570255360D-05
 1.450346070D-08-3.334499340D-12              1.071780920D+05 4.054904945D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10566.089
-1.695114960D+05-8.066262300D+02 8.002802110D+00-1.577046370D-04 2.566205510D-08
-2.403303040D-12 1.676899420D-16              1.154384480D+05-2.133550265D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10566.089
-8.363802520D+07 5.332328580D+04-5.619197890D+00 1.491117690D-03-7.551013120D-08
 1.793856660D-12-1.626371090D-17              -3.111131390D+05 9.671722525D+01
COOH            Cons&Hf298: TPIS,1991,pt1,p60.
 2 tpis91 C   1.00O   2.00H   1.00    0.00    0.00 0   45.0174400    -213000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10813.349
-1.128672450D+04 3.775595570D+02-5.994863920D-01 2.181958800D-02-2.426014210D-05
 1.451317200D-08-3.596447960D-12              -2.841062510D+04 2.934689320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10813.349
 9.293066990D+05-4.483000510D+03 1.242196800D+01-7.463018170D-04 1.332969990D-07
-1.282684930D-11 5.137915590D-16              -8.520206950D+02-5.068046080D+01
CP              TPIS, vol 2, part 1,1989,p35,231-33.
 2 g 7/95 C   1.00P   1.00    0.00    0.00    0.00 0   42.9844610     520158.802
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8715.301
-4.515454470D+04 7.749605360D+02-1.450413330D+00 1.397160140D-02-1.624247050D-05
 9.515561070D-09-2.211986800D-12              5.793069360D+04 3.309536473D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8715.301
-5.646862020D+06 1.736280710D+04-1.633059930D+01 1.143347750D-02-2.821316480D-06
 3.294258940D-10-1.483500100D-14              -4.872316550D+04 1.480113451D+02
CS              TPIS, vol 2, part 1,1989,p35,206-209.
 2 g 7/95 C   1.00S   1.00    0.00    0.00    0.00 0   44.0767000     279771.878
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8708.378
-4.924913220D+04 8.167065760D+02-1.543051900D+00 1.380339350D-02-1.574429060D-05
 9.169869810D-09-2.169745660D-12              2.879872980D+04 3.308573528D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8708.378
-9.719612000D+05 2.339209060D+03 1.709385110D+00 1.577180030D-03-4.146333730D-07
 4.504746640D-11-5.945360240D-16              1.695710240D+04 1.874054728D+01
CS2             TPIS, vol 2, part 1,1991,p28,209-11,NRRAO1.
 2 g 6/95 C   1.00S   2.00    0.00    0.00    0.00 0   76.1427000     116700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10664.223
 1.613287080D+04-4.649089020D+02 6.297719750D+00 1.889507853D-03 3.022885468D-07
-1.736969474D-09 7.791985120D-13              1.477742331D+04-9.302131970D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10664.223
-1.390420939D+06 3.354970030D+03 3.019263826D+00 2.876423317D-03-9.076756730D-07
 1.374080885D-10-6.999507190D-15              -1.013895456D+04 1.565106491D+01
C2              Gurvich et.al.1991,v2,pt1,pp9-14,pt2,pp8-9.8/93
 3 tpis91 C   2.00    0.00    0.00    0.00    0.00 0   24.0214000     830457.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10169.000
 5.559567570D+05-9.980006220D+03 6.681539910D+01-1.743411727D-01 2.448493560D-04
-1.703447061D-07 4.684471300D-11              1.445863861D+05-3.448188920D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10169.000
-9.688909570D+05 3.560990200D+03-5.063511690D-01 2.945092805D-03-7.139289080D-07
 8.670470060D-11-4.076816700D-15              7.681860000D+04 3.339896056D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10169.000
 6.316167420D+06 1.365344126D+04-3.996723210D+00 1.937523033D-03-1.584418225D-07
 5.520765550D-12-7.253609690D-17              9.392905260D+03 6.614126766D+01
C2+             Gurvich et.al. Vol 2, Pt 2, 1991, p 10.
 3 tpis91 C   2.00E  -1.00    0.00    0.00    0.00 0   24.0208514    2004775.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8685.000
-9.913336660D+04 1.347158072D+03-3.476728100D+00 1.676413196D-02-1.865890595D-05
 1.091124814D-08-2.434893253D-12              2.335455402D+05 4.406593746D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8685.000
 3.836171460D+06-6.241787120D+03 2.779000370D+00 6.065908790D-03-2.452804002D-06
 3.882944100D-10-2.190640357D-14              2.857429114D+05 7.311800550D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8685.000
 4.993341380D+07-2.017683043D+04 6.343044090D+00 6.368816330D-04-1.036683912D-07
 4.943005480D-12-7.988437020D-17              4.121156150D+05-2.113730774D+01
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C2-             Gurvich et.al. Vol 2, Pt 2,1991,p 12.
 2 tpis91 C   2.00E   1.00    0.00    0.00    0.00 0   24.0219486     480767.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8676.000
-1.181913390D+05 1.438171226D+03-3.196087470D+00 1.465529260D-02-1.545517062D-05
 9.061115930D-09-2.135933745D-12                4.965329360D+04 4.225547447D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8676.000
 4.478264210D+06-1.154180873D+04 1.310179719D+01-1.862958415D-03 4.014839360D-08
 3.709051950D-11-3.336619040D-15                1.325378956D+05-6.976262583D+01
C2CL            TPIS, vol 2, part 1,1991,p39,112-13.
 2 tpis91 C   2.00CL  1.00    0.00    0.00    0.00 0   59.4741000     534083.071
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10780.626
 4.725995920D+04-8.980386080D+02 9.016973430D+00-6.334065210D-03 1.087103219D-05
-8.089396850D-09 2.248372832D-12                6.702223380D+04-2.354948612D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10780.626
 2.137017514D+05-1.630430045D+03 8.623407160D+00-4.253167720D-04 9.039349620D-08
-1.007494325D-11 4.570759910D-16                7.171034730D+04-2.412955465D+01
C2CL2           TPIS, vol 2, part 1,1991,p43,114.
 2 tpis91 C   2.00CL  2.00    0.00    0.00    0.00 0   94.9268000     200000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14592.612
 3.870154330D+04-9.335408060D+02 1.119295560D+01-3.743959150D-03 6.766954560D-06
-4.907685410D-09 1.298240572D-12                2.628160616D+04-3.310269336D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14592.612
 2.961482255D+05-2.044167935D+03 1.187518625D+01-5.114564140D-04 1.072576584D-07
-1.183353838D-11 5.326531100D-16                3.316798880D+04-4.000745746D+01
C2CL3           TPIS, vol 2, part 1,1991,p52,114-15.
 2 tpis91 C   2.00CL  3.00    0.00    0.00    0.00 0  130.3795000     190271.591
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16150.257
 4.674450170D+04-8.850173190D+02 9.031776930D+00 1.242266156D-02-1.554833695D-05
 9.515574980D-09-2.341986715D-12                2.495823244D+04-1.778799833D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16150.257
-2.203570165D+05-1.073085495D+03 1.378388266D+01-3.094635681D-04 6.781714690D-08
-7.733762500D-12 3.570511430D-16                2.431119041D+04-4.342310230D+01
C2CL4           TPIS, vol 2, part 1,1991,p54,115-16.
 2 tpis91 C   2.00CL  4.00    0.00    0.00    0.00 0  165.8322000     -11000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19605.642
 3.746265540D+04-8.481709630D+02 1.009147436D+01 1.845502653D-02-2.390978804D-05
 1.514902728D-08-3.841381190D-12               -1.072561712D+01-2.368038217D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19605.642
-3.002311850D+05-1.132137810D+03 1.683044135D+01-3.287315830D-04 7.216916110D-08
-8.240017990D-12 3.807379570D-16               -7.069552060D+02-5.979956926D+01
C2CL6           TPIS, vol 2, part 1,1991,p54,117-18.
 2 tpis91 C   2.00CL  6.00    0.00    0.00    0.00 0  236.7376000    -141500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       27129.390
 1.593528070D+05-2.606803543D+03 2.028069734D+01 1.769205442D-02-3.132867373D-05
 2.389211700D-08-6.892464260D-12               -8.231675020D+03-7.953396930D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       27129.390
-5.575766480D+05-4.979882710D+02 2.237066427D+01-1.478456864D-04 3.258021740D-08
-3.726074050D-12 1.722508736D-16               -2.254411904D+04-8.381920380D+01
C2F             TPIS, vol 2, part 1,1991,p39,81-82.
 2 tpis91 C   2.00F   1.00    0.00    0.00    0.00 0   43.0198032     353847.482
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10367.036
 1.249638390D+04-3.483651810D+02 5.754961500D+00 8.531987770D-04 2.353085255D-06
-2.804419370D-09 9.082727790D-13                4.281514500D+04-6.436536051D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10367.036
 2.898780324D+05-2.016654368D+03 8.875066340D+00-5.167005460D-04 1.092156667D-07
-1.212329332D-11 5.483052500D-16                5.241293230D+04-2.773105522D+01
C2FCL           TPIS, vol 2, part 1,1991,p43,141-42.
 2 tpis91 C   2.00F   1.00CL  1.00    0.00    0.00 0   78.4725032      33766.399
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13876.507
 2.698213892D+04-7.415200280D+02 9.630064940D+00-3.878881070D-04 3.005392945D-06
-2.711771879D-09 7.742417850D-13                5.500999360D+03-2.516030804D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13876.507
 3.471343290D+05-2.348439488D+03 1.206875206D+01-5.804827440D-04 1.212825113D-07
-1.334427786D-11 5.994223860D-16                1.502045984D+04-4.252442064D+01
C2FCL3          TPIS, vol 2, part 1,1991,p54,145-46.
 2 tpis91 C   2.00F   1.00CL  3.00    0.00    0.00 0  149.3779032    -166000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18731.914
 1.237204342D+04-4.703874560D+02 7.581589450D+00 2.305730871D-02-2.792142228D-05
 1.679693061D-08-4.077540130D-12               -2.031338422D+04-9.274455340D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18731.914
-2.830419579D+05-1.473622602D+03 1.707856340D+01-4.264066060D-04 9.354057400D-08
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-1.067492645D-11 4.930817980D-16              -1.738583785D+04-6.196890865D+01
C2F2            TPIS, vol 2, part 1,1991,p43,82-83.
 2 tpis91 C   2.00F   2.00    0.00    0.00    0.00 0   62.0182064    -144665.688
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13266.418
 1.776561190D+04-6.113648250D+02 8.663819230D+00 9.150219090D-04 2.364757561D-06
-2.754489635D-09 8.716226650D-13              -1.649593558D+04-2.165268962D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13266.418
 4.192773320D+05-2.715029927D+03 1.230366114D+01-6.647234510D-04 1.384654422D-07
-1.519949190D-11 6.814950940D-16              -4.181326310D+03-4.670120602D+01
C2F2CL2          TPIS,1991. 1,1, cis, trans isomers in eql.
 2 tpis91 C   2.00F   2.00CL  2.00    0.00    0.00 0  132.9236064    -337837.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17936.029
-1.150432931D+05 2.032112631D+03-1.119749346D+01 8.342447530D-02-1.163697872D-04
 7.833086400D-08-2.070001971D-11              -5.208256410D+04 8.888316086D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17936.029
-8.702058680D+05 7.263190890D+02 1.530706863D+01 3.044600749D-04-7.042586530D-08
 8.281840600D-12-3.896343510D-16              -5.208791320D+04-4.998428824D+01
C2F3            TPIS, vol 2, part 1,1991,p52,83-84.
 2 tpis91 C   2.00F   3.00    0.00    0.00    0.00 0   81.0166096    -228181.093
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14163.567
-2.614589241D+04 2.101484587D+02 2.328793094D+00 2.368893664D-02-2.416355046D-05
 1.224857608D-08-2.488496562D-12              -3.028553204D+04 1.699515367D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14163.567
-1.242925975D+05-2.137201615D+03 1.455041017D+01-6.093284240D-04 1.331239775D-07
-1.514837756D-11 6.982427770D-16              -1.977204276D+04-5.420967232D+01
C2F3CL           TPIS, vol 2, part 1,1991,p54,142-43.
 2 tpis91 C   2.00F   3.00CL  1.00    0.00    0.00 0  116.4693096    -515200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17128.149
-8.122992510D+03-1.573931402D+02 5.041785740D+00 2.621694017D-02-2.842996936D-05
 1.537636335D-08-3.360699230D-12              -6.354053870D+04 2.792444988D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17128.149
-2.161888941D+05-2.195350628D+03 1.759632568D+01-6.284019290D-04 1.374527879D-07
-1.565448860D-11 7.220371050D-16              -5.514951580D+04-6.922128665D+01
C2F4            Tetrafluoroethylene. TPIS, vol 2, part 1,1991,p54,84-85.
 2 tpis91 C   2.00F   4.00    0.00    0.00    0.00 0  100.0150128    -659500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16330.554
-9.991359330D+03-1.291148377D+02 4.504284450D+00 2.592007878D-02-2.630267750D-05
 1.316453418D-08-2.624894815D-12              -8.090444590D+04 3.273947372D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16330.554
-1.629348913D+05-2.604072169D+03 1.788508072D+01-7.398181580D-04 1.614807200D-07
-1.836339003D-11 8.460642670D-16              -7.006264750D+04-7.454306600D+01
C2F6            Pentafluoroethyl. TPIS, vol 2, part 1,1991,p54,86-87.
 2 tpis91 C   2.00F   6.00    0.00    0.00    0.00 0  138.0118192   -1344000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20272.040
-3.796232660D+04 7.999522170D+02-4.672262880D+00 7.501647860D-02-9.812408460D-05
 6.320026680D-08-1.622662383D-11              -1.675217831D+05 5.054147406D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20272.040
-1.011461523D+06-9.424720070D+02 2.202582595D+01-1.316098843D-04 1.870581514D-08
-3.473558030D-12 2.491852857D-16              -1.657417898D+05-9.302367534D+01
C2H             Ethynyl. Delh: Ervin,JACS v112,1990. Jacox, 1988.
 2 g 1/91 C   2.00H   1.00    0.00    0.00    0.00 0   25.0293400     566205.472
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10454.472
 7.653691050D+03-4.187401320D+02 7.254271880D+00-5.037019330D-03 8.235196230D-06
-4.616768240D-09 9.509263200D-13              6.850689670D+04-1.586035582D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10454.472
 3.995864090D+06-1.196909290D+04 1.713833040D+01-3.336959570D-03 6.003281300D-07
-5.497240120D-11 2.022731880D-15              1.431423170D+05-9.285925892D+01
C2HCL           TPIS, vol 2, part 1,1991,p43,129.
 2 tpis91 C   2.00H   1.00CL  1.00    0.00    0.00 0   60.4820400     212856.775
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11788.381
 1.329743656D+05-2.174483972D+03 1.497949137D+01-1.290257155D-02 1.602472732D-05
-9.151151360D-09 2.020965585D-12              3.441886730D+04-5.958062406D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11788.381
 1.152211658D+06-4.461391050D+03 1.281389516D+01-6.798637480D-04 1.151764344D-07
-1.047201856D-11 3.953062860D-16              5.071186920D+04-5.320818676D+01
C2HCL3          TPIS, vol 2, part 1,1991,p54,134.
 2 tpis91 C   2.00H   1.00CL  3.00    0.00    0.00 0  131.3874400     -19100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16604.624
 3.958665050D+04-5.177954390D+02 5.154588690D+00 2.817044598D-02-3.624923770D-05
 2.392213529D-08-6.362830250D-12              -1.727164798D+03 1.211816758D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16604.624
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 6.049450330D+05-4.237085160D+03 1.846287907D+01-8.138203680D-04 1.551563178D-07
-1.585216842D-11 6.704638160D-16              1.829097830D+04-7.698468360D+01
C2HF          TPIS, vol 2, part 1,1991,p43,99-100.
 2 tpis91 C   2.00H   1.00F   1.00    0.00    0.00 0   44.0277432     41692.304
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11445.908
 9.160712190D+04-1.537180403D+03 1.133628846D+01-4.623724560D-03 5.876511270D-06
-2.689902086D-09 3.521528050D-13              1.085871558D+04-4.023795008D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11445.908
 1.234330392D+06-4.819538190D+03 1.302333516D+01-7.495242450D-04 1.285409748D-07
-1.184513671D-11 4.536607370D-16              3.236783200D+04-5.640762798D+01
C2HFCL2       TPIS, vol 2, part 1,1991,p102,155-57.
 2 tpis91 C   2.00H   1.00F   1.00CL  2.00    0.00 0  114.9331432    -168648.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16259.290
 3.117108411D+04-1.369095354D+02 1.176176850D+00 4.080836690D-02-5.418223010D-05
 3.613661540D-08-9.626034840D-12              -2.115162595D+04 2.146556135D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16259.290
 4.071761890D+05-3.808350820D+03 1.821160000D+01-7.279824800D-04 1.381775200D-07
-1.405683074D-11 5.921881880D-16              -2.675911299D+03-7.567469866D+01
C2HF2CL       TPIS, vol 2, part 1,1991,p102,153-55.
 2 tpis91 C   2.00H   1.00F   2.00CL  1.00    0.00 0   98.4788464    -333654.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15262.754
 1.704393681D+05-1.667174810D+03 4.788448190D+00 4.444923530D-02-7.322334760D-05
 5.629449630D-08-1.654668362D-11              -3.291839580D+04-5.786711388D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15262.754
 5.830291200D+05-3.810287840D+03 1.798999204D+01-5.887955190D-04 1.002778981D-07
-9.148523660D-12 3.459252710D-16              -2.205893730D+04-7.590922147D+01
C2HF3         TPIS, vol 2, part 1,1991,p54,105.
 2 tpis91 C   2.00H   1.00F   3.00    0.00    0.00 0   82.0245496    -491000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14327.512
-1.411468689D+04 3.688329710D+02-1.145183492D+00 3.956411760D-02-4.602155760D-05
 2.785264108D-08-6.904100370D-12              -6.226444210D+04 3.289875696D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14327.512
 6.917079650D+05-5.260221760D+03 1.915269470D+01-1.072462918D-03 2.099207968D-07
-2.195052735D-11 9.472408220D-16              -3.247692920D+04-8.750405174D+01
CHCO,ketyl      JPCRD v11,sup2,1982. Burcat,TAE 504,Dec 1982.
 2 g 6/89 C   2.00H   1.00O   1.00    0.00    0.00 0   41.0287400     161084.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11239.131
 5.595270450D+04-9.134409630D+02 8.582835480D+00-4.245448560D-03 7.210490290D-06
-3.429508090D-09 4.096335540D-13              2.233853070D+04-2.100792218D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11239.131
 2.154213190D+06-7.508892220D+03 1.407902640D+01-1.256929540D-03 2.236252750D-07
-2.137790230D-11 8.492460770D-16              6.456478340D+04-6.504951868D+01
C2H2,vinylidene   Chen,JCP,v91,1989. Osamura,JACS,v103,1981.
 2 g12/89 C   2.00H   2.00    0.00    0.00    0.00 0   26.0372800     414788.168
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10874.168
-1.465949870D+04 2.789342020D+02 1.276304780D+00 1.394994490D-02-1.475671890D-05
 9.476073440D-09-2.567538140D-12              4.736114160D+04 1.658180626D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10874.168
 1.940844950D+06-6.892744540D+03 1.339586220D+01-9.369202140D-04 1.470875020D-07
-1.220139820D-11 4.122908150D-16              9.107126600D+04-6.337532444D+01
C2H2,acetylene    TPIS 1978. DelH - TRC w-3040, 10/31/88.
 2 g 1/91 C   2.00H   2.00    0.00    0.00    0.00 0   26.0372800     228200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10005.839
 1.598133250D+05-2.216675050D+03 1.265725610D+01-7.980170140D-03 8.055801510D-06
-2.433944610D-09-7.509454610D-14              3.712633790D+04-5.244440564D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10005.839
 1.713792120D+06-5.928970950D+03 1.236115640D+01 1.314706250D-04-1.362869040D-07
 2.712746060D-11-1.302086850D-15              6.266489730D+04-5.818872934D+01
C2H2CL2       TPIS,1991,p102,130-33. 1,1, cis, and trans in equil.
 2 tpis91 C   2.00H   2.00CL  2.00    0.00    0.00 0   96.9426800      3410.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14882.477
-1.203774009D+04 4.629097590D+02-1.318218625D+00 3.930458150D-02-4.851540260D-05
 3.178418750D-08-8.476956350D-12              -3.251839140D+03 3.489235494D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14882.477
 1.561078805D+06-7.357982020D+03 2.011857540D+01-1.310921323D-03 2.411740316D-07
-2.383987226D-11 9.784566740D-16              4.122126890D+04-9.550169906D+01
C2H2FCL       TPIS,1991, 1,1, cis, and trans isomers in eql.
 2 tpis91 C   2.00H   2.00F   1.00CL  1.00    0.00 0   80.4883832    -165082.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13469.313
 2.260141265D+05-2.557412494D+03 9.236168120D+00 2.879423583D-02-5.163988280D-05
 4.252194070D-08-1.311611816D-11              -8.180708670D+03-3.234746746D+01
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13469.313
 1.527659307D+06-6.689630690D+03 1.950545828D+01-1.040881996D-03 1.780488279D-07
-1.632972198D-11 6.212838340D-16                1.705213316D+04-9.194021576D+01
C2H2F2          TPIS,1991,p101-102; 1,1, cis, and trans in equil.
 2 tpis91 C   2.00H   2.00F   2.00    0.00    0.00 0   64.0340864    -336400.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12479.683
 5.702825730D+04-6.762704130D+02 4.117325880D+00 1.822642082D-02-6.861665790D-06
-3.295514650D-09 2.180895828D-12               -3.838658280D+04 1.487993112D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12479.683
-8.228021030D+05-2.915493308D+03 1.830140501D+01-1.039510010D-03 2.546406089D-07
-3.157157655D-11 1.551323183D-15               -3.110174211D+04-8.400665971D+01
CH2CO,ketene     JPCRD,V11,SUP2,1982. JCP v38 1963 p2816.
 2 g 5/90 C   2.00H   2.00O   1.00    0.00    0.00 0   42.0366800     -47700.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11797.743
 3.509613660D+04-4.010302690D+02 3.695982230D+00 1.588572270D-02-1.732648350D-05
 1.161238010D-08-3.314337100D-12               -5.010669530D+03 2.824173220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11797.743
 2.015808050D+06-8.201898320D+03 1.759096140D+01-1.460626760D-03 2.685172740D-07
-2.651861740D-11 1.087321600D-15                4.201636500D+04-8.836982852D+01
C2H3,vinyl       Ervin, JACS 1990, v112, p5750. P.R.Taylor,NASA Ames.
 2 g 2/92 C   2.00H   3.00    0.00    0.00    0.00 0   27.0452200     299740.151
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10575.049
-1.447959530D+04 8.143043440D+02-5.313331680D+00 3.761243250D-02-4.598225990D-05
 3.104721220D-08-8.579917290D-12                3.162346700D+04 5.162588734D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10575.049
 2.561698630D+06-1.005794660D+04 1.851874450D+01-1.719194470D-03 3.093760600D-07
-2.991991430D-11 1.202326250D-15                9.575874480D+04-9.818485136D+01
C2H3CL          TPIS, vol 2, part 1,1991,p54,129-30.
 2 tpis91 C   2.00H   3.00CL  1.00    0.00    0.00 0   62.4979200      23000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11819.647
-1.689084887D+04 8.545357200D+02-6.515097240D+00 4.944715150D-02-6.117802370D-05
 4.067326280D-08-1.101401919D-11               -1.949172611D+03 5.928506220D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11819.647
 2.456166380D+06-1.047449391D+04 2.178733041D+01-1.816874904D-03 3.296321440D-07
-3.214325270D-11 1.302213972D-15                6.358236970D+04-1.149888460D+02
C2H3F           TPIS, vol 2, part 1,1991,p54,100-101.
 2 tpis91 C   2.00H   3.00F   1.00    0.00    0.00 0   46.0436232    -140100.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11335.928
-4.579190090D+04 1.411549115D+03-1.021504673D+01 5.775826220D-02-7.080690630D-05
 4.640860080D-08-1.240458603D-11               -2.402792421D+04 7.860847861D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11335.928
 2.478832992D+06-1.075933774D+04 2.194799679D+01-1.869137086D-03 3.395362220D-07
-3.315516890D-11 1.345164006D-15                4.563463660D+04-1.180412489D+02
CH3CN            Methyl Cyanide.Spangenberg,Z.P.C v255,1974. TRC w9270.
 2 g12/92 C   2.00H   3.00N   1.00    0.00    0.00 0   41.0519600      64430.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12093.105
-9.876195420D+04 1.719390530D+03-7.743314310D+00 4.241840130D-02-4.419036190D-05
 2.658851230D-08-6.863873110D-12               -1.614119440D+03 6.770260616D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12093.105
 2.931022010D+06-1.236540030D+04 2.326673310D+01-2.421350120D-03 4.647007670D-07
-4.774208170D-11 2.029415730D-15                8.052064300D+04-1.294026158D+02
CH3CO,acetyl     Hf:JPC v96 1992 p5881. Cons:JACS v111 1989 p7675
 2 g 6/96 C   2.00H   3.00O   1.00    0.00    0.00 0   43.0446200     -10000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13036.467
-7.194006080D+04 1.464481049D+03-6.632364460D+00 4.108493140D-02-4.226293830D-05
 2.485795570D-08-6.292648090D-12               -9.309446970D+03 6.422944588D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13036.467
 2.485510168D+06-1.120747766D+04 2.277560881D+01-2.314445154D-03 4.536692510D-07
-4.743321170D-11 2.045030478D-15                6.380304740D+04-1.215376745D+02
C2H4             JPCRD v4,75,p251. Ch.Phys,v98,85,p1. Hf298:TRCw-2600 4/88.
 2 g 1/91 C   2.00H   4.00    0.00    0.00    0.00 0   28.0531600      52500.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10518.689
-1.163613270D+05 2.554860520D+03-1.609750300D+01 6.625786370D-02-7.885086390D-05
 5.125223790D-08-1.370338460D-11               -6.176236060D+03 1.093340298D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10518.689
 3.408725120D+06-1.374836420D+04 2.365884830D+01-2.423728560D-03 4.431169150D-07
-4.352348400D-11 1.775218290D-15                8.820356340D+04-1.371268982D+02
C2H4O,ethylen-o   Ethylene oxide. NSRDS-NBS 39 1972. JANAF JPCRD v14 sup1 1985.
 2 g 8/88 C   2.00H   4.00O   1.00    0.00    0.00 0   44.0525600     -52634.720
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10830.615
-1.728240240D+05 3.816688750D+03-2.629857540D+01 1.014104720D-01-1.240580700D-04
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 8.034058340D-08-2.120948140D-11              -2.437524090D+04 1.654887942D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10830.615
 3.151847330D+06-1.423657620D+04 2.708093580D+01-2.606312030D-03 4.854102420D-07
-4.852436590D-11 2.011933290D-15              7.662633220D+04-1.563961968D+02
CH3CHO,ethanal    Chao,JPCRD,1986,v.15,p1369.  TRC for Hf, Jn,1978.
 2 g 8/88 C   2.00H   4.00O   1.00    0.00    0.00 0   44.0525600    -166190.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12896.716
-1.373921920D+05 2.559961270D+03-1.340482360D+01 5.922159980D-02-6.240049210D-05
 3.703354960D-08-9.342785090D-12              -3.318742770D+04 1.007424322D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12896.716
 3.321164640D+06-1.449717890D+04 2.708420170D+01-2.879317900D-03 5.556308300D-07
-5.732673100D-11 2.443963140D-15              6.507741160D+04-1.536235338D+02
CH3COOH          Acetic acid. JPCRD vol 7, NO 1, 1978, P 363.
 2 g 8/88 C   2.00H   4.00O   2.00    0.00    0.00 0   60.0519600    -432249.040
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13597.325
-3.219214970D+04 1.196319640D+03-8.705813310D+00 5.696259140D-02-5.757891910D-05
 3.352119470D-08-8.614451970D-12              -5.840107520D+04 7.282403862D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13597.325
 2.103541150D+06-1.467832430D+04 3.382815920D+01-5.694937410D-03 1.343245220D-06
-1.606076280D-10 7.652992930D-15              2.924291340D+04-1.935288240D+02
C2H5             Chen,JCP v93 no2,Jul90,p1191.
 2 g12/92 C   2.00H   5.00    0.00    0.00    0.00 0   29.0611000     118658.240
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12185.244
-1.411328380D+05 2.714311820D+03-1.534990770D+01 6.451706200D-02-7.259191320D-05
 4.599150570D-08-1.218377740D-11              5.980117710D+02 1.090973590D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12185.244
 4.169208950D+06-1.662979570D+04 2.795440300D+01-3.051710670D-03 5.685158670D-07
-5.682879040D-11 2.355665840D-15              1.137008370D+05-1.639356890D+02
C2H5Br           Bromoethane. TRC tuvw7650 6/30/1979
 2 x 6/79 C   2.00H   5.00BR  1.00    0.00    0.00 0  108.9651000     -63600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13569.000
-1.374172641D+05 2.861429359D+03-1.824108925D+01 8.566230520D-02-1.047174460D-04
 6.906074470D-08-1.862275992D-11              -2.198480178D+04 1.258435395D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13569.000
 2.378652344D+06-1.267034389D+04 2.777559362D+01-2.010902219D-03 4.436092070D-07
-5.348209040D-11 2.639841317D-15              6.414066900D+04-1.528277775D+02
C2H6             Ethane.  JPCRD VOL 11, NO 1, P 83, 1982.
 2 g 8/88 C   2.00H   6.00    0.00    0.00    0.00 0   30.0690400     -83851.544
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11891.594
-1.862050300D+05 3.406200690D+03-1.951710090D+01 7.565850030D-02-8.204196030D-05
 5.061154460D-08-1.319288080D-11              -2.702937110D+04 1.298142962D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11891.594
 5.025809410D+06-2.033030460D+04 3.322562120D+01-3.836754150D-03 7.238549960D-07
-7.319384490D-11 3.065579950D-15              1.115969080D+05-2.039417458D+02
CH3N2CH3         Azomethane. JPCRD vol 11 no 1,1982,p83.
 2 g 8/88 C   2.00H   6.00N   2.00    0.00    0.00 0   58.0825200     148699.360
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16524.999
-3.738481710D+05 5.880433850D+03-2.986385080D+01 1.087376300D-01-1.167942270D-04
 6.916827900D-08-1.719928170D-11              -1.189975300D+04 1.948239010D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16524.999
 4.993354460D+06-2.160998460D+04 3.964455930D+01-4.196499780D-03 8.023543620D-07
-8.212562030D-11 3.477423730D-15              1.449963770D+05-2.372113860D+02
C2H5OH           Ethanol. CHAO,JPCRD,NO4,1986,p1369.  Hf, TRC 6/87.
 2 g 8/88 C   2.00H   6.00O   1.00    0.00    0.00 0   46.0684400    -234950.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14541.926
-2.342810005D+05 4.479205560D+03-2.744830238D+01 1.088682495D-01-1.305313938D-04
 8.437379230D-08-2.234568547D-11              -5.022241150D+04 1.764836305D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14541.926
 4.694781590D+06-1.929789472D+04 3.447575990D+01-3.236129500D-03 5.784860890D-07
-5.564495220D-11 2.226175096D-15              8.601565200D+04-2.034795998D+02
CH3OCH3          DIMETHYL ETHER. CHAO,JPCRD,NO4,1986. Hf298,TRC W-6040.
 2 g12/92 C   2.00H   6.00O   1.00    0.00    0.00 0   46.0684400    -184110.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14354.432
-2.693081970D+05 4.300692310D+03-2.152782330D+01 8.131833910D-02-8.295688300D-05
 4.801931630D-08-1.188707170D-11              -4.410228070D+04 1.467663620D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14354.432
 4.933577310D+06-2.083094380D+04 3.629052420D+01-4.108366270D-03 7.903269900D-07
-8.131512640D-11 3.458211500D-15              1.013301180D+05-2.185448150D+02
CCN              CCN RAD. f: TPIS 1991. Jacox 1988.
 2 g12/92 C   2.00N   1.00    0.00    0.00    0.00 0   38.0281400     804803.412
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11245.464
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-1.795266430D+04 1.445770260D+02 3.613635840D+00 5.747522550D-03-2.879649400D-06
-1.703276530D-10 4.088280390D-13                9.460381510D+04 6.957871588D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11245.464
 9.117680060D+04-1.382903380D+03 8.372619490D+00-2.687685720D-04 3.516279880D-08
-5.694034170D-13-8.399674210D-17                1.025813060D+05-2.278441154D+01
CNC             Cnc rad. Constants & Hf298; TPIS V.2,PT 1,1991
 2 tpis91 C   2.00N   1.00    0.00    0.00    0.00 0   38.0281400     684917.118
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11359.170
-7.081487720D+04 1.008442400D+03-1.579046540D+00 2.052862630D-02-2.279223490D-05
 1.283501750D-08-2.933460370D-12                7.612866100D+04 3.488780866D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11359.170
-9.032753160D+04-8.309529390D+02 8.114337920D+00-2.445515800D-04 5.391262620D-08
-6.175085200D-12 2.860233200D-16                8.451661200D+04-2.102380564D+01
C2N2            Gurvich et.al., VOL 2, PART 2, 1979, P 220.
 2 tpis79 C   2.00N   2.00    0.00    0.00    0.00 0   52.0348800     309100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12715.000
 1.082391272D+05-1.928114409D+03 1.553873056D+01-1.821136999D-02 2.778806789D-05
-1.899411060D-08 4.949616810D-12                4.449088660D+04-6.090893850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12715.000
 7.950631520D+05-4.001900810D+03 1.314975564D+01-8.774079250D-04 2.066532979D-07
-2.210686446D-11 1.002915169D-15                5.866544020D+04-5.476696130D+01
C2O             Constants & Hf298: TPIS 1979. Jacox, 1988.
 2 g12/89 C   2.00O   1.00    0.00    0.00    0.00 0   40.0208000     291039.367
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10486.419
-2.440762710D+03-1.349636610D+02 4.733266350D+00 3.299802210D-03-8.829276680D-08
-1.780483330D-09 7.826612790D-13                3.421061260D+04-3.017906352D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10486.419
 3.254887820D+05-2.339535720D+03 9.741595400D+00-1.245633460D-03 3.758635360D-07
-5.077046050D-11 2.541249850D-15                4.660045220D+04-3.300689278D+01
C3              Props&Hf: TPIS,v2,pt2,1979,p23.
 3 tpis79 C   3.00    0.00    0.00    0.00    0.00 0   36.0321000     839948.500
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12109.000
-4.354562850D+04 6.660104140D+02 1.451015130D+00 7.434425310D-03-3.810109540D-06
-2.336756050D-11 4.406996310D-13                9.635174010D+04 2.025141786D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12109.000
 4.508043980D+06-1.461016000D+04 2.281947010D+01-8.544236920D-03 2.146043290D-06
-2.103842140D-10 6.351511060D-15                1.911964920D+05-1.271855040D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12109.000
 5.621956270D+08-4.800148200D+05 1.487736040D+02-1.863807580D-02 1.253693450D-06
-4.231520540D-11 5.696510730D-16                3.777690200D+06-1.226349444D+03
C3H3,1-propynl    TRC tuvw-3140 4/98. Extrapolated.
 2 x 4/98 C   3.00H   3.00    0.00    0.00    0.00 0   39.0559200     450000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12400.000
-6.505859350D+04 1.350858921D+03-5.825433930D+00 3.756610480D-02-3.734903340D-05
 2.117676603D-08-5.139113250D-12                4.656510530D+04 5.781470636D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12400.000
 4.550654870D+06-1.640574172D+04 2.712605991D+01-4.474600380D-03 1.037712415D-06
-1.250211369D-10 6.026582050D-15                1.534087662D+05-1.565932501D+02
C3H3,2-propynl    TRC tuvw-3140 4/98. Extrapolated.
 2 x 4/98 C   3.00H   3.00    0.00    0.00    0.00 0   39.0559200     331800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.000
 6.188578320D+04-8.909578670D+02 6.347558820D+00 1.633173115D-02-1.949975695D-05
 1.417349778D-08-4.199866320D-12                4.271785830D+04-1.231407643D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13230.000
 2.989723833D+06-1.118954446D+04 2.222225052D+01-2.068106902D-03 4.121883640D-07
-4.438980590D-11 1.970824701D-15                1.061878289D+05-1.186745275D+02
C3H4,allene       TRC w-2750,1984. Shimanouchi,1972. J.Raman Spec.v1,1973
 2 g12/92 C   3.00H   4.00    0.00    0.00    0.00 0   40.0638600     190920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12604.569
-1.645617210D+04 9.630126460D+02-7.532704630D+00 5.518326130D-02-6.733745950D-05
 4.532831170D-08-1.251874370D-11                1.772462330D+04 6.152215610D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12604.569
 3.479262900D+06-1.430386960D+04 2.702507540D+01-2.557268860D-03 4.706253560D-07
-4.651155460D-11 1.907938630D-15                1.072295940D+05-1.548822884D+02
C3H4,propyne      TRC w-3000. JCP v18,1950,p1613. NSRDS-NBS v39,1972,p116
 2 g12/92 C   3.00H   4.00    0.00    0.00    0.00 0   40.0638600     184510.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13030.516
-3.563923470D+04 8.328186360D+02-4.073780570D+00 4.113934070D-02-4.470449930D-05
 2.847461280D-08-7.695307070D-12                1.705513290D+04 4.516729540D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13030.516
 3.710430050D+06-1.489142860D+04 2.732394750D+01-2.645253220D-03 4.858266620D-07
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-4.794074230D-11 1.964303100D-15                1.104427650D+05-1.567991084D+02
C3H4,cyclo-       Cyclopropene.JPCRD v15 n2,1986,p437.
 2 g 5/90 C   3.00H   4.00    0.00    0.00    0.00 0   40.0638600     277100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11373.663
-1.969799800D+04 1.505418000D+03-1.418227280D+01 7.642688180D-02-9.765661920D-05
 6.612060150D-08-1.811267350D-11                2.625613120D+04 9.604744420D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11373.663
 3.168385270D+06-1.371042550D+04 2.664303230D+01-2.420414280D-03 4.428028790D-07
-4.351883580D-11 1.775987460D-15                1.133682140D+05-1.522618954D+02
C3H5,allyl        Mol.Data-Bur92.  Hf298-JPCRD v.20 no2,1991,pp 221-273.
 2 bur 92 C   3.00H   5.00    0.00    0.00    0.00 0   41.0718000     169000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14066.725
-1.241314160D+05 2.245573540D+03-1.177844880D+01 6.222613590D-02-6.763506160D-05
 4.178431060D-08-1.092426660D-11                8.381324140D+03 9.106975636D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14066.725
 3.978759950D+06-1.687426370D+04 3.142456780D+01-3.306813750D-03 6.341627620D-07
-6.506121380D-11 2.759847340D-15                1.196433600D+05-1.818181298D+02
C3H6,propylene    Mol.data- JPCRD v4,1975,p251. Hform- TRC 4/30/88,w2600.
 2 g 2/95 C   3.00H   6.00    0.00    0.00    0.00 0   42.0797400      20000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13550.558
-1.912452970D+05 3.542059670D+03-2.114869610D+01 8.901457300D-02-1.001424830D-04
 6.267926120D-08-1.637860850D-11               -1.529955000D+04 1.407636138D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13550.558
 5.017620820D+06-2.086084840D+04 3.644157930D+01-3.881202540D-03 7.278715300D-07
-7.321264290D-11 3.052212020D-15                1.261245800D+05-2.195717162D+02
C3H6,cyclo-       JPCRD v15 n2,1986,p437. J.MolSp v47,1973,64-83.
 2 g 1/93 C   3.00H   6.00    0.00    0.00    0.00 0   42.0797400      53300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11409.981
-1.565846810D+05 4.111214060D+03-3.233494260D+01 1.306350920D-01-1.645583210D-04
 1.095722960D-07-2.956438810D-11               -1.245312040D+04 1.931584798D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11409.981
 4.784990800D+06-2.042117480D+04 3.631496960D+01-3.561332880D-03 6.476290740D-07
-6.328506510D-11 2.568747870D-15                1.268273480D+05-2.223730112D+02
C3H6O             Propylene oxide. Various refs.
 2 g 6/90 C   3.00H   6.00O   1.00    0.00    0.00 0   58.0791400     -93720.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14405.391
-2.292837570D+05 4.495781870D+03-2.941135460D+01 1.213118330D-01-1.440066420D-04
 9.202091490D-08-2.416288970D-11               -3.317712350D+04 1.846887046D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14405.391
 4.789694050D+06-2.106886990D+04 3.954638750D+01-3.910885240D-03 7.325418060D-07
-7.356949600D-11 3.060559580D-15                1.120338660D+05-2.371998654D+02
C3H7,n-propyl     Mole.data- Tsang,JACS May 1985, p 2872.
 2 g 6/90 C   3.00H   7.00    0.00    0.00    0.00 0   43.0876800     100500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14860.058
-1.895344270D+05 3.949527910D+03-2.606222050D+01 1.121922040D-01-1.365294410D-04
 9.023677410D-08-2.441060740D-11               -7.227928200D+03 1.673708564D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14860.058
 5.646500410D+06-2.291085090D+04 3.987274890D+01-4.106241430D-03 7.562608850D-07
-7.478368720D-11 3.069058300D-15                1.483005370D+05-2.403781096D+02
C3H7,i-propyl     Mol.data- Tsang,JACS May 1985, p 2872.
 2 g 9/85 C   3.00H   7.00    0.00    0.00    0.00 0   43.0876800      93300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14807.207
-2.952086370D+05 5.294465870D+03-3.105306090D+01 1.143876950D-01-1.291760430D-04
 8.057904500D-08-2.093926690D-11               -1.476831520D+04 1.988092614D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14807.207
 5.806950760D+06-2.411207970D+04 4.085278410D+01-4.517814010D-03 8.499366210D-07
-8.573485540D-11 3.583396500D-15                1.546496060D+05-2.487091186D+02
C3H8              TRC w1350,10/85. JPCRD V2,NO2,1973,P427.
 2 g 6/90 C   3.00H   8.00    0.00    0.00    0.00 0   44.0956200    -104680.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14742.059
-2.431722550D+05 4.653455400D+03-2.937377870D+01 1.188288030D-01-1.375333190D-04
 8.807975650D-08-2.341112880D-11               -3.539084140D+04 1.840640638D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14742.059
 6.421429170D+06-2.660017570D+04 4.534512970D+01-5.021256480D-03 9.472478000D-07
-9.576809280D-11 4.010308060D-15                1.455729810D+05-2.818493672D+02
C3H8O,1propanol   Props&Hf298: TRC,6/87.  1500K+:JPCRD v15,1986,p1369.
 2 g 9/88 C   3.00H   8.00O   1.00    0.00    0.00 0   60.0950200    -255200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17462.000
-2.504063910D+05 5.035210970D+03-3.226173120D+01 1.345966050D-01-1.591423600D-04
 1.023128600D-07-2.708189140D-11               -5.536875210D+04 2.041842320D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17462.000
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 5.460837770D+06-2.396117150D+04 4.459816290D+01-3.384566870D-03 5.398451340D-07
-4.645636800D-11 1.636616470D-15                1.097188200D+05-2.673969080D+02
C3H8O,2propanol   Hf298: TRC 6/87. Cons: JPCRD v15,1986,p1369.
 2 g 9/88 C   3.00H   8.00O   1.00    0.00    0.00 0   60.0950200    -272700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17264.183
-3.388721400D+05 6.109384700D+03-3.793337360D+01 1.530989610D-01-1.864963810D-04
 1.213623580D-07-3.221301260D-11                -6.281535420D+04 2.335386800D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17264.183
 6.000115500D+06-2.505623720D+04 4.621928220D+01-4.271835430D-03 7.692316870D-07
-7.449018050D-11 2.998219080D-15                1.148350040D+05-2.796004630D+02
C3O2            Carbon suboxide. Hf298:JANAF6/68. Cons:JPCRD v6,'77p993.
 2 g 7/88 C   3.00O   2.00    0.00    0.00    0.00 0   68.0309000     -93640.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15084.982
 1.579801970D+05-2.529380990D+03 1.801691670D+01-1.785814060D-02 2.978313580D-05
-2.182605450D-08 6.012848200D-12                -1.121821730D+03-7.277342638D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15084.982
 6.967137570D+05-4.624315240D+03 1.663862450D+01-1.175265330D-03 2.477520780D-07
-2.744408090D-11 1.239190050D-15                1.252285660D+04-7.275657328D+01
C4              Cons & Hf: TPIS,v2,pt1,1979,p21.
 2 g 7/88 C   4.00    0.00    0.00    0.00    0.00 0   48.0428000    1033903.742
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13117.742
 3.903189110D+04-8.947397790D+02 1.050901570D+01-6.551407780D-03 1.243714120D-05
-8.643613460D-09 2.263118910D-12                1.266421680D+05-3.077315034D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13117.742
 9.200962920D+05-1.530402500D+03 6.050184540D+00 5.252671590D-03-1.779131660D-06
 2.589837630D-10-1.385532000D-14                1.334395290D+05-7.261998182D+00
C4H2            1,3-Butadiyne. Thermochim.Acta,v178,1991,p273.
 2 g 2/93 C   4.00H   2.00    0.00    0.00    0.00 0   50.0586800     450000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14393.860
 2.467515870D+05-3.897817240D+03 2.366059020D+01-2.208018280D-02 2.781014150D-05
-1.577275950D-08 3.422978090D-12                7.086889440D+04-1.109162010D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14393.860
 2.328169460D+06-8.925163000D+03 2.114325540D+01-1.368873620D-03 2.327542960D-07
-2.124620510D-11 8.054111580D-16                1.057786850D+05-1.088312820D+02
C4H4,1,3-cyclo-   1,3-Cyclobutadiene.JPCRD v15 n2,1986,p437.
 2 g 5/90 C   4.00H   4.00    0.00    0.00    0.00 0   52.0745600     385000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12103.534
-2.778502850D+04 1.768186910D+03-1.757900200D+01 9.383524950D-02-1.195525760D-04
 7.978095280D-08-2.152753350D-11                3.811622250D+04 1.128480638D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12103.534
 2.991530650D+06-1.416793040D+04 3.001994060D+01-2.579292730D-03 4.790268890D-07
-4.775731490D-11 1.975144580D-15                1.274674070D+05-1.727543092D+02
C4H6,butadiene    1,3-butadiene.TRC,Oct 31,1992,tuvw-2820,extrapolated.
 2 x10/92 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     110000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15130.000
-9.181129690D+04 3.312570430D+03-2.985828550D+01 1.479201130D-01-2.056618300D-04
 1.466496810D-07-4.145285680D-11                -2.077308950D+03 1.780686634D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15130.000
-2.361903470D+07 5.651324100D+04-3.275739000D+01 2.293070890D-02-2.297107250D-06
 4.292606290D-11 4.236761050D-15               -3.671359100D+05 3.013437134D+02
C4H6,1-butyne     TRC tables, Oct 31,1993, tuvw-3040. Extrapolated.
 2 x10/93 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     165200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16020.000
-5.597039600D+04 1.433191660D+03-9.691210450D+00 7.150002320D-02-8.157967700D-05
 5.290364890D-08-1.435655350D-11                1.184987040D+04 7.660218554D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16020.000
 4.032213880D+06-1.907255490D+04 3.832573160D+01-3.941266950D-03 9.171304900D-07
-1.134588360D-10 5.657333090D-15                1.301733360D+05-2.252740506D+02
C4H6,2-butyne     TRC tables, Oct 31,1993, tuvw-3040. Extrapolated.
 2 x10/93 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     145700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16640.000
-2.650756420D+05 4.490728710D+03-2.400723900D+01 9.819579580D-02-1.079717190D-04
 6.675555810D-08-1.740766900D-11                -5.328363810D+03 1.595034604D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16640.000
 3.790405230D+06-1.821626850D+04 3.603987300D+01-2.145243200D-03 3.525913580D-07
-3.222481650D-11 1.247197540D-15                1.228119640D+05-2.118773016D+02
C4H6,cyclo-       Cyclobutene.JPCRD v15 n2,1986,p437.
 2 g 5/90 C   4.00H   6.00    0.00    0.00    0.00 0   54.0904400     156700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12557.564
-2.046731490D+05 4.919504040D+03-3.753296470D+01 1.497298060D-01-1.860146840D-04
 1.219914750D-07-3.254091420D-11                -3.916111420D+03 2.233292014D+02
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12557.564
 4.517319220D+06-2.097302080D+04 4.008032690D+01-3.949781470D-03 7.448509000D-07
-7.529861060D-11 3.153346630D-15                1.406463100D+05-2.434832246D+02
C4H8,1-butene     TRC tuvw-2600, Apr.30,1988.
 2 x 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200       -540.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17120.000
-2.721491800D+05 5.100079010D+03-3.183786110D+01 1.317754400D-01-1.527359280D-04
 9.714760690D-08-2.560204350D-11                -2.523096270D+04 2.006931388D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17120.000
 1.246644290D+07-4.523771370D+04 6.909674730D+01-1.634502100D-02 4.079621450D-06
-5.099743240D-10 2.504147180D-14                2.753715330D+05-4.446484892D+02
C4H8,cis2-buten   TRC tuvw-2600, Apr.30,1988.
 2 x 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200      -7400.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16800.000
-2.773870550D+05 5.382383620D+03-3.375187860D+01 1.322980560D-01-1.490975820D-04
 9.277721260D-08-2.408282730D-11                -2.715884140D+04 2.114461308D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16800.000
 1.196419810D+07-4.414503760D+04 6.735510230D+01-1.522655630D-02 3.739449400D-06
-4.616277520D-10 2.244819570D-14                2.674043520D+05-4.342233882D+02
C4H8,tr2-butene   TRC tuvw-2600, Apr.30,1988.
 2 x 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200     -11000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17510.000
-3.594644000D+05 5.930971920D+03-3.255825200D+01 1.254957750D-01-1.374705330D-04
 8.407341070D-08-2.163047260D-11                -3.113296450D+04 2.070080528D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17510.000
 1.334962960D+07-4.834917920D+04 7.286467810D+01-1.855070670D-02 4.742020150D-06
-6.052554190D-10 3.024941540D-14                2.935637790D+05-4.729021062D+02
C4H8,isobutene    TRC tuvw-2600, Apr.30,1988.
 2 x 4/88 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200     -17100.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17010.000
-2.327204930D+05 3.941994020D+03-2.224581070D+01 1.012790830D-01-1.073194020D-04
 6.454696540D-08-1.646330240D-11                -2.233765960D+04 1.479596918D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17010.000
 1.475252310D+07-5.234908320D+04 7.747002510D+01-2.121745970D-02 5.531511520D-06
-7.169714460D-10 3.626215830D-14                3.184241060D+05-5.059505142D+02
C4H8,cyclo-       Cyclobutane. JPCRD v15 n2,1986,p437.
 2 g 5/90 C   4.00H   8.00    0.00    0.00    0.00 0   56.1063200      28400.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13534.163
-3.047655820D+05 6.519482520D+03-4.662987470D+01 1.743593020D-01-2.090964130D-04
 1.343528640D-07-3.542727290D-11                -2.700031070D+04 2.738347488D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13534.163
 4.456210650D+06-2.301017710D+04 4.492447700D+01-3.080141460D-03 5.317155660D-07
-5.081066940D-11 2.048912750D-15                1.355487090D+05-2.771802052D+02
(CH3COOH)2        (acetic acid)2.JPCRD v7 n1,p363,1978.
 2 g 6/90 C   4.00H   8.00O   4.00    0.00    0.00 0  120.1039200    -929015.360
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        28053.457
-3.094787970D+05 5.983484960D+03-3.573058940D+01 1.662537440D-01-1.883880340D-04
 1.154948090D-07-2.935188700D-11                -1.421500780D+05 2.295887870D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        28053.457
 6.571343940D+06-3.036877860D+04 6.250390990D+01-5.732734500D-03 1.083501110D-06
-1.098030660D-10 4.609695490D-15                6.347470020D+04-3.734564890D+02
C4H9,n-butyl      TRC tables, tuvw-1940, Oct.31,1984.
 2 x10/84 C   4.00H   9.00    0.00    0.00    0.00 0   57.1142600      66530.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19797.000
-2.239560410D+05 4.676554110D+03-2.985424450D+01 1.345493700D-01-1.600660350D-04
 1.045338100D-07-2.812951050D-11                -1.525297710D+04 1.901650930D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19797.000
 1.257009460D+07-4.572090150D+04 7.099502200D+01-1.580928930D-02 3.913036270D-06
-4.857024540D-10 2.372837060D-14                2.859689670D+05-4.541400720D+02
C4H9,i-butyl      2-methylethyl. TRC tables, tuvw-1940, Oct.31,1984.
 2 x10/84 C   4.00H   9.00    0.00    0.00    0.00 0   57.1142600      57320.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18317.000
-2.399461230D+05 4.697444450D+03-3.087472510D+01 1.391655820D-01-1.670233950D-04
 1.092423070D-07-2.936209920D-11                -1.638150990D+04 1.936661710D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18317.000
 8.297503790D+06-3.296621130D+04 5.662869240D+01-7.849618640D-03 1.670785560D-06
-1.842000030D-10 8.216641090D-15                2.035826100D+05-3.523799200D+02
C4H9,s-butyl      1-methylpropyl rad.  Tsang, JACS, v107, no.10, p2872.
 2 g 1/93 C   4.00H   9.00    0.00    0.00    0.00 0   57.1142600      71000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17537.648
-3.351050330D+05 6.312928070D+03-4.003015160D+01 1.563872120D-01-1.842327260D-04
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 1.182724370D-07-3.131146200D-11              -2.216037100D+04 2.481289820D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17537.648
 7.224663580D+06-3.035272420D+04 5.288536790D+01-5.652032790D-03 1.060027030D-06
-1.066133570D-10 4.443892080D-15              1.883481840D+05-3.255708820D+02
C4H9,t-butyl      1,1-dimethylethyl. Tsang, JACS, v107, no.10, p2872.
 2 g 1/93 C   4.00H   9.00    0.00    0.00    0.00 0   57.1142600     51700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17009.675
-4.723479630D+05 8.090227780D+03-4.683693940D+01 1.575306050D-01-1.686569540D-04
 9.981126310D-08-2.487637720D-11              -3.319380900D+04 2.894848470D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17009.675
 7.150931100D+06-3.171188370D+04 5.442473060D+01-6.392141480D-03 1.241047130D-06
-1.287181050D-10 5.512266240D-15              1.934483700D+05-3.399298600D+02
C4H10,isobutane   TRC w-1350,10/85. JPCRD v4 n4,1975,p859.
 2 g 6/90 C   4.00H  10.00    0.00    0.00    0.00 0   58.1222000   -134990.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17936.501
-3.834479540D+05 7.000049080D+03-4.440028800D+01 1.746182970D-01-2.078193210D-04
 1.339789920D-07-3.551672050D-11              -5.034023970D+04 2.658967590D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17936.501
 7.527789560D+06-3.202457370D+04 5.700101200D+01-6.059715190D-03 1.143897650D-06
-1.156958930D-10 4.845509210D-15              1.728462000D+05-3.576133700D+02
C4H10,n-butane    TRC w 1350,10/85. JPCRD v4 n4,1975,p859.
 2 g 6/90 C   4.00H  10.00    0.00    0.00    0.00 0   58.1222000   -125790.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19228.783
-3.175783260D+05 6.176159710D+03-3.891428550D+01 1.584612410D-01-1.859990630D-04
 1.199636030D-07-3.201564450D-11              -4.540288060D+04 2.379417520D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19228.783
 7.682227690D+06-3.256026940D+04 5.736700430D+01-6.197729820D-03 1.180131500D-06
-1.221815330D-10 5.250196000D-15              1.774510960D+05-3.587896170D+02
C4N2              2-Butynedinitrile. JANAF Mar. 1978.
 2 j 3/61 C   4.00N   2.00    0.00    0.00    0.00 0   76.0562800    533460.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17734.459
 1.489213950D+05-2.815826690D+03 2.243583670D+01-2.375052190D-02 3.837867070D-05
-2.736703030D-08 7.370359360D-12              7.478097610D+04-9.594164814D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17734.459
 1.026263520D+06-5.887561880D+03 2.045610280D+01-1.470016240D-03 3.080616210D-07
-3.396892170D-11 1.528312470D-15              9.504729810D+04-9.541320894D+01
C5                Cons & Hf: TPIS,v2,pt1,1979,p21.
 2 g 7/88 C   5.00    0.00    0.00    0.00    0.00 0   60.0535000   1050924.331
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16191.831
-1.201135320D+04-5.553218060D+02 1.123800970D+01-4.347121690D-03 1.738875560D-05
-1.707863450D-08 5.574306140D-12              1.262402310D+05-3.262161254D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16191.831
 2.172469480D+05-2.958657780D+03 1.561099540D+01-8.201415420D-04 1.777188440D-07
-2.010231200D-11 9.224518350D-16              1.395217260D+05-6.433212764D+01
C5H6,1,3cyclo-    1,3-Cyclopentadiene. Pedley 1986. Dorfeeva, 1986.
 2 g 5/90 C   5.00H   6.00    0.00    0.00    0.00 0   66.1011400    134300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13535.529
-1.016694080D+05 3.484818670D+03-3.187887800D+01 1.472153880D-01-1.854244950D-04
 1.226113520D-07-3.286862560D-11              3.292455560D+02 1.890531260D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13535.529
 4.448856560D+06-2.128443550D+04 4.314408720D+01-3.936254990D-03 7.364942360D-07
-7.393423240D-11 3.077087900D-15              1.385758920D+05-2.609328310D+02
C5H8,cyclo-       Cyclopentene. JPCRD v15 n2,1986,p437. TRC w-2840.
 2 g 1/93 C   5.00H   8.00    0.00    0.00    0.00 0   68.1170200     33900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14857.179
-2.631114420D+05 5.987753240D+03-4.522244460D+01 1.804626300D-01-2.177216000D-04
 1.402022630D-07-3.699094170D-11              -2.379504630D+04 2.660135670D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14857.179
 4.569864860D+06-2.406022520D+04 4.881010520D+01-3.413074590D-03 6.047051640D-07
-5.927559690D-11 2.447897620D-15              1.413985860D+05-2.989537160D+02
C5H10,1-pentene   TRC tables tuvw-2500, Apr.30,1987.
 2 x 4/87 C   5.00H  10.00    0.00    0.00    0.00 0   70.1329000    -21280.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21680.000
-5.340547930D+05 9.298917060D+03-5.667792270D+01 2.123100210D-01-2.571298210D-04
 1.666834250D-07-4.434080300D-11              -4.790682030D+04 3.396035658D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21680.000
 4.536789700D+06-2.483775240D+04 5.316138090D+01-4.122243540D-03 9.899756050D-07
-1.246788240D-10 6.289971180D-15              1.381412870D+05-3.188524162D+02
C5H10,cyclo-      Cyclopentane. JPCRD v15 n2,1986,p437.
 2 g 6/90 C   5.00H  10.00    0.00    0.00    0.00 0   70.1329000    -78400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15023.337
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-4.141124870D+05 8.627597610D+03-6.202961200D+01 2.259910880D-01-2.682302910D-04
 1.706289520D-07-4.464049870D-11              -4.947160020D+04 3.583916728D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15023.337
 7.501820610D+06-3.505834380D+04 6.322450020D+01-6.940198150D-03 1.337262920D-06
-1.377844270D-10 5.867025500D-15                1.953342160D+05-4.026528932D+02
C5H11,pentyl      TRC tables tuvw-1941, Oct.31,1984.
 2 x10/84 C   5.00H  11.00    0.00    0.00    0.00 0   71.1408400      45810.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24422.000
-4.653715880D+05 8.564220490D+03-5.295242920D+01 2.094288870D-01-2.561602920D-04
 1.692755970D-07-4.596788140D-11              -3.641704300D+04 3.196861628D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24422.000
 1.245272720D+07-4.927235910D+04 8.165797890D+01-1.681409650D-02 4.195315910D-06
-5.223498900D-10 2.551358700D-14                3.009986820D+05-5.203809782D+02
C5H11,t-pentyl    1,1-dimethylpropyl rad. Tsang,JACS,v107 n10,1985,p2872.
 2 g 1/93 C   5.00H  11.00    0.00    0.00    0.00 0   71.1408400      32600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19643.723
-5.152197160D+05 9.144354210D+03-5.602415680D+01 1.998210110D-01-2.239122910D-04
 1.375464560D-07-3.523863880D-11              -4.036278730D+04 3.402820238D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19643.723
 8.601872900D+06-3.805143820D+04 6.649627970D+01-7.533550860D-03 1.451532390D-06
-1.495488700D-10 6.367487060D-15                2.281818590D+05-4.169363482D+02
C5H12,n-pentane   TRC tables. Oct 31,1985. tuvw 1350.
 2 x10/85 C   5.00H  12.00    0.00    0.00    0.00 0   72.1487800    -146760.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24184.000
-3.324925380D+05 6.564507110D+03-3.982378580D+01 1.623256680D-01-1.646102000D-04
 8.968870420D-08-1.994705410D-11              -5.022307920D+04 2.472552956D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24184.000
 6.212257350D+06-3.212578450D+04 6.406353370D+01-5.307076630D-03 1.151357030D-06
-1.354791010D-10 6.538086750D-15                1.667252640D+05-3.960858384D+02
C5H12,i-pentane   2-Methylbutane. TRC tables. Oct 31,1985. tuvw 1350.
 2 x10/85 C   5.00H  12.00    0.00    0.00    0.00 0   72.1487800    -153700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22008.000
-4.231903290D+05 6.497189020D+03-3.681126920D+01 1.532424720D-01-1.548790700D-04
 8.749896980D-08-2.070547670D-11              -5.155416550D+04 2.309517566D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22008.000
 8.502517220D+06-3.711142790D+04 6.638139420D+01-3.869728750D-03 5.635713710D-07
-4.857318650D-11 1.871459880D-15                1.999038350D+05-4.176271144D+02
CH3C(CH3)2CH3     2,2-Dimethypropane (neopentane) TRC tuvw 1130,10/85.
 2 x10/85 C   5.00H  12.00    0.00    0.00    0.00 0   72.1487800    -167920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23179.000
-8.973221990D+06 1.289225580D+05-7.199344610D+02 2.056862120D+00-2.953159610D-03
 2.158893080D-06-6.268318580D-10              -6.394931840D+05 4.020806178D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23179.000
 1.684729130D+07-5.979489150D+04 8.685506850D+01-9.622178390D-03 1.653427950D-06
-1.674809140D-10 7.372521920D-15                3.458535220D+05-5.760508184D+02
C6H2            Hf298 & Cons: Thermochimica Acta,v178,1991,p273.
 2 g 2/93 C   6.00H   2.00    0.00    0.00    0.00 0   74.0800800     670000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19607.713
 2.903817040D+05-4.929883080D+03 3.189394400D+01-3.119640120D-02 4.326041870D-05
-2.732721240D-08 6.675045190D-12                1.011905020D+05-1.530633148D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19607.713
 2.592801450D+06-1.083351630D+04 2.847452000D+01-1.876708160D-03 3.412138050D-07
-3.337476050D-11 1.356938250D-15                1.418510330D+05-1.494848078D+02
C6H5,phenyl       NASA TM 83800, 1985. TRC 10/89.
 2 g 1/91 C   6.00H   5.00    0.00    0.00    0.00 0   77.1039000     337200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14004.788
-1.602341950D+05 3.937489250D+03-3.200327550D+01 1.437285760D-01-1.742524290D-04
 1.110877070D-07-2.889361150D-11              2.207106430D+04 1.933058990D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14004.788
 3.767622460D+06-1.953125830D+04 4.227424440D+01-3.698464730D-03 7.001532290D-07
-7.106308110D-11 2.987541100D-15                1.512441310D+05-2.515103280D+02
C6D5,phenyl       NASA TM-83800, 1985.
 2 G12/84 C   6.00D   5.00    0.00    0.00    0.00 0   82.1347100     306947.830
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.254978200D+00 4.732876600D-02-8.075988300D-06
-2.990197200D-08 1.714906000D-11              3.531406300D+04 2.978008026D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.472949200D+01 1.521053500D-02-5.524163500D-06
 8.798457500D-10-5.097921700D-14              3.028262900D+04-5.575502974D+01
C6H5O,phenoxy     NASA TM-83800, 1985.
 2 g 6/90 C   6.00H   5.00O   1.00    0.00    0.00    0.00 0   93.1033000      47697.600
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16208.093
-1.292267810D+05 3.406745390D+03-2.911369640D+01 1.459180890D-01-1.780203350D-04
 1.138616310D-07-2.967143710D-11              -1.055057930D+04 1.770683030D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16208.093
 3.678627400D+06-1.972978510D+04 4.541183330D+01-3.751064660D-03 7.114464480D-07
-7.233360680D-11 3.045658480D-15                1.163591460D+05-2.681057920D+02
C6H6            NASA TM 83800, 1985. TRC 10/86.
 2 g 1/91 C   6.00H   6.00    0.00    0.00    0.00 0   78.1118400     82880.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14194.791
-1.682826540D+05 4.412514520D+03-3.722063930D+01 1.641918150D-01-2.023219880D-04
 1.309662940D-07-3.448887830D-11              -1.039254320D+04 2.172442068D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14194.791
 4.549770270D+06-2.261533940D+04 4.692207200D+01-4.196808220D-03 7.870297270D-07
-7.919216430D-11 3.303430000D-15                1.392388400D+05-2.867689812D+02
C6D6            NASA TM-83800, 1985.
 2 G12/84 C   6.00D   6.00    0.00    0.00    0.00 0   84.1488120     58177.984
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.070121800D+00 5.293819700D-02-9.607482800D-06
-3.280237200D-08 1.901252800D-11                5.406898400D+03 3.069380883D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.561986400D+01 1.712393400D-02-6.201275900D-06
 9.849305800D-10-5.689155700D-14              -1.443305200D+02-6.388825317D+01
C6H5OH,phenol     NASA TM 83800, JAN 1985.
 2 g 6/90 C   6.00H   6.00O   1.00    0.00    0.00 0   94.1112400    -96399.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17496.669
-1.209487160D+05 3.378413220D+03-2.991927870D+01 1.567827200D-01-1.970971040D-04
 1.291837940D-07-3.424412170D-11              -2.779442100D+04 1.799752756D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17496.669
 4.462031210D+06-2.165507850D+04 4.815005730D+01-3.568247820D-03 6.327105630D-07
-6.039831920D-11 2.399136290D-15                1.113717470D+05-2.860447664D+02
C6H10,cyclo-      Cyclohexene. JPCRD v15 n2,1986,p437.
 2 g 1/93 C   6.00H  10.00    0.00    0.00    0.00 0   82.1436000     -4600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17270.784
-3.750313080D+05 7.643911880D+03-5.510448360D+01 2.166233360D-01-2.545452400D-04
 1.607605590D-07-4.185238410D-11              -3.661090830D+04 3.202417322D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17270.784
 7.510055180D+06-3.556837590D+04 6.703012760D+01-7.045233950D-03 1.358134050D-06
-1.400030820D-10 5.964323610D-15                2.060261070D+05-4.238182008D+02
C6H12,1-hexene    TRC tuvw-2500,Apr 30, 1987.
 2 x 4/87 C   6.00H  12.00    0.00    0.00    0.00 0   84.1594800    -41950.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26240.000
-6.692505780D+05 1.180232740D+04-7.289547270D+01 2.714479400D-01-3.340589200D-04
 2.187691750D-07-5.874880500D-11              -6.231940530D+04 4.297157128D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26240.000
 5.055636740D+06-2.797896870D+04 6.193418560D+01-4.298110380D-03 1.062869270D-06
-1.354835130D-10 6.864810810D-15                1.525160740D+05-3.721089662D+02
C6H12,cyclo-      Cyclohexane. JPCRD v15 n2,1986,p437.
 2 g 6/90 C   6.00H  12.00    0.00    0.00    0.00 0   84.1594800   -123300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17544.814
-5.680043000D+05 1.034245590D+04-6.800072460D+01 2.387804300D-01-2.511897050D-04
 1.425296570D-07-3.407838700D-11              -6.404669350D+04 3.934825968D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17544.814
 5.224978700D+06-3.364153530D+04 7.174569730D+01-6.698802650D-03 1.318397610D-06
-1.390732070D-10 6.059748120D-15                1.732510570D+05-4.546786732D+02
C6H13,n-hexyl     TRC tuvw-1930,Oct 31, 1983.
 2 x10/83 C   6.00H  13.00    0.00    0.00    0.00 0   85.1674200     25100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       28983.000
-1.427278210D+06 2.248828080D+04-1.297492230D+02 4.279797300D-01-5.556013140D-04
 3.791256910D-07-1.048462400D-10              -1.060261010D+05 7.497186076D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       28983.000
 1.337192210D+07-5.571055840D+04 9.552021830D+01-1.962122430D-02 5.015681540D-06
-6.381959110D-10 3.180369770D-14                3.345756110D+05-6.095258964D+02
C6H14,n-hexane    TRC tuvw-1440,4/85. JCP v60 n8,p3144,1974. W extrap.
 2 g 6/96 C   6.00H  14.00    0.00    0.00    0.00 0   86.1753600   -166920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       28702.000
-5.815926540D+05 1.079097705D+04-6.633946920D+01 2.523715124D-01-2.904344659D-04
 1.802201480D-07-4.617223580D-11              -7.271544480D+04 3.938282854D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       28702.000
 1.795732742D+07-6.681221210D+04 1.062781853D+02-2.260964619D-02 5.738738360D-06
-7.345701080D-10 3.705109780D-14                3.840326600D+05-6.912454836D+02
C7H7,benzyl       Hippler JPC v94,1990,p3803.  JPC v92,1988,p4905.
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 2 g 1/93 C   7.00H   7.00    0.00    0.00    0.00 0   91.1304800     210500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18554.892
-1.836735330D+05 4.102415430D+03-3.202372950D+01 1.588238810D-01-1.894448900D-04
 1.203634860D-07-3.136542630D-11                5.266565090D+03 1.938733498D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18554.892
 5.297206150D+06-2.599879280D+04 5.509720790D+01-4.977514540D-03 9.462780090D-07
-9.638541010D-11 4.064240480D-15                1.738363320D+05-3.343808042D+02
C7H8            Various references.
 2 g 1/93 C   7.00H   8.00    0.00    0.00    0.00 0   92.1384200      50170.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17940.345
-2.878036950D+05 6.134047380D+03-4.574765210D+01 1.936911920D-01-2.304329260D-04
 1.459319180D-07-3.790849990D-11               -2.308453310D+04 2.693947216D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17940.345
 6.184514650D+06-2.990279800D+04 5.982003770D+01-5.696982640D-03 1.080750530D-06
-1.098708100D-10 4.624786350D-15                1.782044890D+05-3.698080794D+02
C7H8O,cresol-mx   Eql mixture. Kudchadker et al JPCRD v7 n2,p417,1978.
 2 g 1/93 C   7.00H   8.00O   1.00    0.00    0.00 0  108.1378200    -132298.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21838.869
-2.443922530D+05 5.084303760D+03-3.790553320D+01 1.865208350D-01-2.269743210D-04
 1.459088110D-07-3.822558980D-11               -4.095343460D+04 2.282250118D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21838.869
 6.017427260D+06-2.849961450D+04 6.081596630D+01-4.997000110D-03 9.134656430D-07
-8.979814920D-11 3.667900340D-15                1.472264970D+05-3.674891252D+02
C7H14,1-heptene   TRC tuvw-2500,Apr 30, 1987.
 2 x 4/87 C   7.00H  14.00    0.00    0.00    0.00 0   98.1860600     -62760.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30790.000
-7.477150500D+05 1.336127080D+04-8.303433680D+01 3.114020690D-01-3.795385000D-04
 2.453104250D-07-6.506823620D-11               -7.236825240D+04 4.868780158D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30790.000
 5.164927020D+06-2.988200350D+04 6.926966900D+01-3.673074330D-03 9.165385290D-07
-1.169994750D-10 5.918814520D-15                1.590155910D+05-4.150995112D+02
C7H15,n-heptyl    TRC tuvw-1930, 10/83
 2 x10/83 C   7.00H  15.00    0.00    0.00    0.00 0   99.1940000       4390.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33543.000
-1.671733520D+06 2.640010270D+04-1.526867720D+02 5.027121440D-01-6.521014070D-04
 4.443488140D-07-1.227815010D-10               -1.273754630D+05 8.783932744D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33543.000
 1.404589550D+07-6.095208000D+04 1.075272640D+02-2.115970460D-02 5.412231870D-06
-6.882155180D-10 3.425583700D-14                3.609964490D+05-6.858382056D+02
C7H16,2-methylh   2-methyl hexane. TRC tuvw-1460,10/31/85
 2 x10/85 C   7.00H  16.00    0.00    0.00    0.00 0  100.2019400    -194600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30920.000
-7.104777950D+05 1.191251140D+04-7.345339550D+01 2.902952400D-01-3.462767720D-04
 2.260184530D-07-6.128814010D-11               -8.202147790D+04 4.320041722D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30920.000
 1.279685210D+07-5.570838910D+04 1.000867970D+02-1.356813280D-02 3.284583890D-06
-4.152821520D-10 2.098969020D-14                3.048121340D+05-6.384029218D+02
C7H16,n-heptane   TRC tuv-1460,10/31/85; p1010,10/31/84.
 2 x10/85 C   7.00H  16.00    0.00    0.00    0.00 0  100.2019400    -187780.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33221.000
-6.127432750D+05 1.184085400D+04-7.487188410D+01 2.918466000D-01-3.416795410D-04
 2.159285210D-07-5.655852550D-11               -8.013408770D+04 4.407212582D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33221.000
 1.281533590D+07-5.412562050D+04 9.801194590D+01-1.382706520D-02 3.432678310D-06
-4.359953720D-10 2.200167280D-14                2.966648740D+05-6.216764368D+02
C8H8,styrene      Ethenylbenzene,TRC Apr 30,1989,tuvw-4490, Extrapolated.
 2 x 4/89 C   8.00H   8.00    0.00    0.00    0.00 0  104.1491200     148300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20940.000
-2.686930400D+05 6.167999270D+03-4.836054830D+01 2.182873200D-01-2.738561790D-04
 1.810084950D-07-4.867750170D-11               -1.140639880D+04 2.817678258D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20940.000
 1.638245270D+06-2.009957370D+04 5.594342140D+01-4.059454300D-03 1.001584120D-06
-1.300825790D-10 6.751798590D-15                1.227484620D+05-3.309262202D+02
C8H10,ethylbenz   Ethylbenzene. TRC Oct 31,1986,tuvw-3200, Extrapolated.
 2 x10/86 C   8.00H  10.00    0.00    0.00    0.00 0  106.1650000      29920.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22280.000
-4.694939900D+05 9.307168030D+03-6.521769300D+01 2.612080190D-01-3.181753410D-04
 2.051355420D-07-5.401817190D-11               -4.073870060D+04 3.780903582D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22280.000
 5.206906880D+06-3.075040760D+04 6.823159500D+01-6.146404170D-03 1.386600340D-06
-1.663556900D-10 8.094217150D-15                1.758731280D+05-4.184631888D+02
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C8H16,1-octene    TRC tuvw-2500,Apr 30, 1987.
 2 x 4/87 C   8.00H  16.00    0.00    0.00    0.00 0  112.2126400     -83590.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       35350.000
-9.313881930D+05 1.645523300D+04-1.018444840D+02 3.754863850D-01-4.600746370D-04
 2.972553470D-07-7.861258640D-11              -8.974253180D+04 5.921548758D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       35350.000
 5.983719610D+06-3.343325130D+04 7.808594280D+01-3.725028310D-03 9.354140380D-07
-1.188982030D-10 5.970371690D-15               1.764151290D+05-4.690149132D+02
C8H17,n-octyl     TRC tuvw-1930,10/83.
 2 x10/83 C   8.00H  17.00    0.00    0.00    0.00 0  113.2205800     -16320.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38103.000
-1.934340970D+06 3.054979780D+04-1.767903430D+02 5.801596580D-01-7.517413900D-04
 5.112468950D-07-1.410193640D-10              -1.498894680D+05 1.013724256D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38103.000
 1.486878860D+07-6.658739270D+04 1.199321360D+02-2.289384430D-02 5.858824560D-06
-7.446289110D-10 3.702955670D-14               3.899710710D+05-7.650445076D+02
C8H18,n-octane    N-octane. TRC tuvw-1490, 4/85.
 2 x 4/85 C   8.00H  18.00    0.00    0.00    0.00 0  114.2285200    -208750.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       37780.000
-6.986647240D+05 1.338501120D+04-8.415166050D+01 3.271936690D-01-3.777209640D-04
 2.339837030D-07-6.010892770D-11              -9.026223360D+04 4.939222120D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       37780.000
 7.872500120D+06-4.264415630D+04 9.214326520D+01-7.011885370D-03 1.731905660D-06
-2.206635570D-10 1.120026530D-14               2.161953360D+05-5.681063670D+02
C8H18,isooctane   2,2,4-Trimethylpentane. TRC tables tuvw-1490,4/30/85.
 2 x 4/85 C   8.00H  18.00    0.00    0.00    0.00 0  114.2285200    -224010.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       32170.000
-1.688758670D+05 3.126903390D+03-2.123502920D+01 1.489151530D-01-1.151180170D-04
 4.473216440D-08-5.554882860D-12              -4.468060690D+04 1.417455210D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       32170.000
 2.538918210D+07-9.131930620D+04 1.387154810D+02-2.273819660D-02 5.274807240D-06
-6.576111640D-10 3.305971790D-14               5.292638330D+05-9.196307610D+02
C9H19,n-nonyl     TRC(10/83)tuvw-1930.
 2 x10/83 C   9.00H  19.00    0.00    0.00    0.00 0  127.2471600     -37030.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       42664.000
-2.194880610D+06 3.468565790D+04-2.009261420D+02 6.580503130D-01-8.525930040D-04
 5.794638980D-07-1.597637100D-10              -1.723194610D+05 1.149113956D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       42664.000
 1.563322120D+07-7.206377910D+04 1.321722090D+02-2.454427080D-02 6.283205040D-06
-7.981043430D-10 3.965093520D-14               4.179193270D+05-8.430570156D+02
C10H8,naphthale   Naphthalene. Chen,JPCFD v8 n2 1979 p527-535.
 2 g 8/93 C  10.00H   8.00    0.00    0.00    0.00 0  128.1705200     150580.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20713.076
-2.602920990D+05 6.237519290D+03-5.226157400D+01 2.397710630D-01-2.912272160D-04
 1.854965710D-07-4.816685340D-11              -1.114753250D+04 2.972172708D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20713.076
 5.905864570D+06-3.163144910D+04 7.030252590D+01-6.018395960D-03 1.141923860D-06
-1.161432010D-10 4.891928210D-15               1.962512700D+05-4.347785692D+02
C10H21,n-decyl    TRC(10/83)tuvw-1930.
 2 x10/83 C  10.00H  21.00    0.00    0.00    0.00 0  141.2737400     -57740.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       47224.000
-2.446511140D+06 3.870081310D+04-2.244388180D+02 7.343624970D-01-9.513525610D-04
 6.462970340D-07-1.781502860D-10              -1.941633890D+05 1.280987776D+03
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       47224.000
 1.648474510D+07-7.779222320D+04 1.446842360D+02-2.633569170D-02 6.745062100D-06
-8.564829550D-10 4.252224410D-14               4.474832370D+05-9.230323448D+02
C12H9,o-bipheny   O-biphenyl. NASA 83800, Jan 1985.
 2 g12/84 C  12.00H   9.00    0.00    0.00    0.00 0  153.1998600     427730.320
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26589.335
-3.595938880D+05 7.661543420D+03-5.873389540D+01 2.697583670D-01-3.229791160D-04
 2.032930280D-07-5.231378890D-11               1.458341970D+04 3.392742106D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26589.335
 6.736160260D+06-3.632114470D+04 8.210157350D+01-7.501916820D-03 1.456134670D-06
-1.506983390D-10 6.435593590D-15               2.555472960D+05-5.042403764D+02
C12D9,o-bipheny   NASA TM-83800, 1985.
 2 G12/84 C  12.00D   9.00    0.00    0.00    0.00 0  162.2553180     386511.721
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-7.329939600D-01 8.983689500D-02-1.373127500D-05
-5.942702000D-08 3.370243000D-11               4.294309400D+04 3.004188944D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.012319900D+01 2.832825500D-02-1.036654000D-05
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 1.659333800D-09-9.652711600D-14                3.320778900D+04-1.351913736D+02
C12H10,biphenyl   NASA 83800, Jan 1985.
 2 g12/84 C  12.00H  10.00    0.00    0.00    0.00 0  154.2078000     182130.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26783.511
-3.671136410D+05 8.128582810D+03-6.391096080D+01 2.901449040D-01-3.509625700D-04
 2.231013340D-07-5.788532400D-11               -1.679342250D+04 3.633520600D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26783.511
 7.480124810D+06-3.928019510D+04 8.661411460D+01-7.946026580D-03 1.531764870D-06
-1.576305200D-10 6.699807990D-15                2.438006660D+05-5.381330710D+02
C12D10,biphenyl   NASA TM-83800, 1985.
 2 G12/84 C  12.00D  10.00    0.00    0.00    0.00 0  164.2694200     138415.822
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00-1.579348600D+00 9.505957400D-02-1.453207100D-05
-6.264559700D-08 3.553007900D-11                1.313742200D+04 3.152977526D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 3.090506000D+01 3.034998800D-02-1.109504800D-05
 1.775581000D-09-1.033232700D-13                2.883445300D+03-1.424390028D+02
Ca              Hf:CODATA 1989. JPCRD v14 sup.2 1985.
 3 g 8/97 CA  1.00    0.00    0.00    0.00    0.00 0   40.0780000     177800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.063892786D+04 4.384548330D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 7.547341240D+06-2.148642662D+04 2.530849567D+01-1.103773705D-02 2.293249636D-06
-1.209075383D-10-4.015333268D-15                1.585862323D+05-1.609512955D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.291781634D+09-1.608862960D+06 4.312466360D+02-5.396508990D-02 3.531856210D-06
-1.164403850D-10 1.527134223D-15                1.258651434D+07-3.692101610D+03
Ca+             Spec:JPCRD v14 sup.2 1985.
 3 g 1/98 CA  1.00E  -1.00    0.00    0.00    0.00 0   40.0774514     773827.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                9.232417790D+04 5.077674980D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.747070820D+06-1.174707738D+04 1.672546969D+01-8.334797710D-03 2.394593294D-06
-2.988243468D-10 1.356563002D-14                1.664329088D+05-9.582821260D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 9.117128410D+08-6.220428460D+05 1.683741136D+02-2.140862670D-02 1.452947686D-06
-4.920790880D-11 6.575369235D-16                4.959472060D+06-1.422600719D+03
CaBr            Props & D0: TPIS 1996 pt1 p471, pt2 p367.
 2 tpis96 CA  1.00BR  1.00    0.00    0.00    0.00 0  119.9820000     -24868.681
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9856.119
 5.693832620D+02-1.257513537D+02 5.001508330D+00-1.039868753D-03 1.377594927D-06
-8.949013960D-10 2.395658928D-13               -3.728103980D+03 1.784864847D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9856.119
 2.783236402D+06-8.458203730D+03 1.431756560D+01-5.430781680D-03 1.522218659D-06
-1.831824807D-10 7.864288660D-15                4.931270680D+04-6.537001100D+01
CaBr2           Hsubl & cons: TPIS v3 pt1 p474; pt2 p369.
 2 tpis96 CA  1.00BR  2.00    0.00    0.00    0.00 0  199.8860000    -387197.300
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15603.200
 1.572504318D+03-2.238551236D+02 8.388457890D+00-1.944164774D-03 2.397926088D-06
-1.556572350D-09 4.124309580D-13               -4.772106610D+04-1.074965233D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15603.200
-2.219846426D+04-4.463155330D+00 7.503755110D+00-1.641654626D-06 3.879428060D-10
-4.683424260D-14 2.259325541D-18               -4.885436820D+04-5.590324250D+00
CaCL            Props & D0: TPIS 1996 pt1 p464, pt2 p363.
 2 tpis96 CA  1.00CL  1.00    0.00    0.00    0.00 0   75.5307000    -103772.885
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9595.115
 6.395335260D+03-2.249042269D+02 5.283278390D+00-1.447983237D-03 1.643742771D-06
-9.430104280D-10 2.237516133D-13               -1.270169000D+04-1.391970247D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9595.115
 1.629182545D+06-4.766223020D+03 9.658929770D+00-2.523044131D-03 5.833542160D-07
-4.101726990D-11 8.813177640D-17                1.662599241D+04-3.398731770D+01
CaCL+           Props & IP: TPIS 1996 pt1 p466, pt2 p364.
 2 tpis96 CA  1.00CL  1.00E  -1.00    0.00    0.00 0   75.5301514     467190.513
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9361.113
 2.285284542D+03-2.002872721D+02 4.936990190D+00-3.860973030D-04 8.686661880D-08
 1.470205680D-10-7.689315870D-14                5.588277950D+04-6.359874920D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9361.113
 1.770280396D+05-5.891372390D+02 5.103368800D+00-2.356761168D-04 5.483732870D-08
 2.137973112D-14-5.572887310D-16                5.853417250D+04-2.191259602D+00
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CaCL2           Hsubl & cons: TPIS v3 pt1 p470; pt2 p366.
 2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 0  110.9834000    -485243.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14857.023
 1.106802030D+04-4.249108250D+02 9.134711860D+00-3.497185310D-03 4.242184630D-06
-2.719673231D-09 7.138268630D-13              -5.850346760D+04-1.808679105D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14857.023
-3.595768780D+04-8.796495630D+00 7.507256910D+00-3.129465934D-06 7.322886480D-10
-8.776403220D-14 4.210486040D-18              -6.066779660D+04-8.553531560D+00
CaF             Props & D0: TPIS 1996 pt1 p456, pt2 p359.
 2 tpis96 CA  1.00F   1.00    0.00    0.00    0.00 0   59.0764032    -276403.790
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9132.110
 3.184235400D+04-4.918235090D+02 5.701120890D+00-1.465138218D-03 9.092930810D-07
-1.367585222D-10-5.106323380D-14              -3.197694110D+04-5.996662260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9132.110
 5.195882670D+05-1.512321567D+03 5.869276250D+00-3.882524480D-04-2.484582298D-08
 3.749915960D-11-3.470976450D-15              -2.488814584D+04-8.614663700D+00
CaF+            Props & IP: TPIS 1996 pt1 p460, pt2 p360.
 2 tpis96 CA  1.00F   1.00E  -1.00    0.00    0.00 0   59.0758546     260664.608
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9003.108
 4.158340800D+04-5.627661660D+02 5.687522150D+00-1.264710572D-03 6.669086480D-07
-6.926752820D-11-3.978714620D-14               3.305119500D+04-6.974485010D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9003.108
-1.398670845D+05 2.191526375D+02 4.214324340D+00 2.142798048D-04-5.778672600D-08
 9.985756310D-12-6.059621880D-16               2.841605897D+04 2.740342729D+00
CaF2            Hsubl0,Cons: TPIS v3 pt1 p462; pt2 p362.
 2 tpis96 CA  1.00F   2.00    0.00    0.00    0.00 0   78.0748064    -790828.409
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12811.591
 5.909352290D+04-1.019733042D+03 1.013165309D+01-5.503506440D-03 5.629319980D-06
-3.115401465D-09 7.205525940D-13              -9.192608190D+04-2.639505950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12811.591
-8.280409440D+04-3.115950071D+01 7.023577370D+00-9.521000020D-06 2.118160895D-09
-2.440713888D-13 1.135135468D-17              -9.729466770D+04-7.546243340D+00
CaH             Props & D0: TPIS 1996 pt1 p447, pt2 p353.
 2 tpis96 CA  1.00H   1.00    0.00    0.00    0.00 0   41.0859400     229409.105
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8705.105
-4.513782230D+04 7.629429210D+02-1.280874223D+00 1.318774659D-02-1.481595334D-05
 8.536573220D-09-1.989958945D-12               2.300378814D+04 3.053421525D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8705.105
-2.696952529D+06 8.607059750D+03-7.027454820D+00 7.467916310D-03-2.318610699D-06
 3.423072420D-10-1.892679792D-14              -2.773819107D+04 7.845822010D+01
CaI             Props & D0: TPIS 1996 pt1 p474, pt2 p370.
 2 tpis96 CA  1.00I   1.00    0.00    0.00    0.00 0  166.9824700      12183.320
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10018.120
-8.261790180D+02-8.508975900D+01 4.864171690D+00-7.863169650D-04 1.100493506D-06
-7.348030610D-10 2.010892767D-13               5.236753440D+02 3.585391680D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10018.120
 1.771071309D+06-5.683643730D+03 1.153857476D+01-4.194020200D-03 1.291359961D-06
-1.730043579D-10 8.380762350D-15               3.583293200D+04-4.405917570D+01
CaI2            Hsubl & cons: TPIS v3 pt1 p477; pt2 p372.
 2 tpis96 CA  1.00I   2.00    0.00    0.00    0.00 0  293.8869400    -259319.505
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16050.995
-1.097851401D+03-1.459821761D+02 8.089341840D+00-1.305332923D-03 1.624199331D-06
-1.061194001D-09 2.825551217D-13              -3.272692980D+04-6.981714940D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16050.995
-1.623727104D+04-2.859530722D+00 7.502432190D+00-1.071178707D-06 2.544559095D-10
-3.083631004D-14 1.491836724D-18              -3.346341170D+04-3.567305740D+00
CaO             Props & D0: TPIS 1996 pt1 p443, pt2 p349.
 3 tpis96 CA  1.00O   1.00    0.00    0.00    0.00 0   56.0774000      38005.308
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8953.108
 3.889733070D+04-4.835677350D+02 5.077713250D+00 3.076235250D-04-1.159759897D-06
 8.493433340D-10-1.495333366D-13               5.937643480D+03-3.955320730D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8953.108
-4.913106170D+07 1.495865950D+05-1.681654149D+02 9.381950260D-02-2.455529428D-05
 3.074980720D-09-1.485914237D-13              -9.461511720D+05 1.235694769D+03
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8953.108
-3.504055130D+08 2.083212387D+05-3.978209270D+01 5.039268720D-03-3.220707680D-07
 1.057379426D-11-1.396044154D-16              -1.662378721D+06 3.934491930D+02
CaO+            Props & Hf0: TPIS 1996 pt1 p445, pt2 p351.
 3 tpis96 CA  1.00O   1.00E  -1.00    0.00    0.00 0   56.0768514     710237.542
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9163.110
 1.098060332D+05-1.459992448D+03 9.880777940D+00-9.157564600D-03 8.707582560D-06
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-4.390411080D-09 9.264854660D-13              9.150057350D+04-3.009947701D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9163.110
 9.397843130D+05-2.993362243D+03 8.336191820D+00-2.303295087D-03 7.373967530D-07
-1.052888279D-10 5.257138410D-15              1.028098401D+05-2.461547836D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9163.110
-7.648645260D+07 1.739245253D+04 8.420288710D+00-1.168386844D-03 8.413684900D-08
-2.770799280D-12 3.569474430D-17              -8.643489770D+04-2.376513061D+01
CaOH            Hf0 & cons: TPIS v3 pt1 p451; pt2 p355.
 2 tpis96 CA  1.00O   1.00H   1.00    0.00    0.00 0   57.0853400    -173307.350
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11049.697
 4.620028900D+04-9.285672820D+02 9.175828770D+00-3.962828800D-03 2.505447308D-06
 3.852068210D-11-3.352778470D-13              -1.798009717D+04-2.533704850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11049.697
 1.979972994D+06-5.598880990D+03 1.151348706D+01-1.668264707D-03 3.312573910D-07
-1.789056647D-11-3.580716410D-16              1.340196822D+04-4.646084260D+01
CaOH+           Hf0 & cons: TPIS v3 pt1 p452; pt2 p356.
 2 tpis96 CA  1.00O   1.00H   1.00E  -1.00    0.00 0   57.0847914     372938.100
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11097.719
 4.884342660D+04-9.832415100D+02 9.610182950D+00-5.204360660D-03 4.263049820D-06
-1.197590878D-09 9.028411890D-15              4.795056340D+04-2.827077334D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11097.719
 8.637615370D+05-2.347302046D+03 7.981911200D+00 1.003160947D-04-6.240074170D-08
 1.019540904D-11-5.698925280D-16              5.830580120D+04-2.152181937D+01
Ca(OH)2         Hf0 & cons: TPIS v3 pt1 p455; pt2 p358.
 2 tpis96 CA  1.00O   2.00H   2.00    0.00    0.00 0   74.0926800    -598338.869
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16592.281
 8.389257540D+04-1.791902135D+03 1.621891031D+01-7.840857170D-03 5.095111610D-06
-6.955487550D-11-6.132152640D-13              -6.600405630D+04-6.070913920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16592.281
 1.721854884D+06-4.702217670D+03 1.396947691D+01 1.983791405D-04-1.243050592D-07
 2.033402404D-11-1.137157819D-15              -4.443761350D+04-5.287444860D+01
CaS             Props & D0: TPIS 1996 pt1 p480, pt2 p374.
 2 tpis96 CA  1.00S   1.00    0.00    0.00    0.00 0   72.1440000     121475.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9360.113
 2.320990615D+04-4.518446080D+02 6.172333750D+00-3.598852020D-03 4.823731710D-06
-3.631733540D-09 1.212849867D-12              1.554597691D+04-7.686915670D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9360.113
-1.568353214D+07 5.293855810D+04-6.322467240D+01 4.027726380D-02-1.114855081D-05
 1.464389344D-09-7.376078970D-14              -3.172022670D+05 4.799606220D+02
Ca2             Props and D0: TPIS 1996 pt1 p439 pt2 p347.
 2 tpis96 CA  2.00    0.00    0.00    0.00    0.00 0   80.1560000     341765.336
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11273.136
-8.582228620D+04 1.588188960D+02 1.103952055D+01-3.333196760D-02 5.345938810D-05
-4.011573240D-08 1.160486682D-11              3.770350800D+04-2.397744561D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11273.136
 2.405966267D+05 5.775803820D+01 2.347436675D+00 1.199275034D-04-4.329150310D-08
 7.015302690D-12-3.705660320D-16              4.081875400D+04 1.895399607D+01
Cd              Hf:CODATA 1989 p25. NSRDS-NBS 35 vIII 1971 p55
 3 g 7/97 CD  1.00    0.00    0.00    0.00    0.00 0  112.4110000     111800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.081751543D-04 1.816433041D-06 2.499999989D+00 3.129989231D-11-4.600710160D-14
 3.407048740D-17-9.989497436D-21              1.270099766D+04 5.931549760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.699757467D+05 7.866001140D+02 1.628169079D+00 4.594123290D-04-1.150420443D-07
 1.074836707D-11 8.790199555D-17              7.675148260D+03 1.220006052D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.336284287D+09 9.320949110D+05-2.490956222D+02 3.302878610D-02-2.200384347D-06
 7.425712550D-11-1.026730246D-15              -7.267528990D+06 2.167946107D+03
Cd+             NSRDS,NBS 35 vIII 1971 p59
 3 g 7/97 CD  1.00E  -1.00    0.00    0.00    0.00 0  112.4104514     985754.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21              1.178129439D+05 6.624689450D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.484880812D+04-4.669153680D+01 2.557883006D+00-3.624701700D-05 1.213747570D-08
-2.072802814D-12 1.420665367D-16              1.181070109D+05 6.216414480D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-6.428364400D+07 4.740395160D+04-1.165755517D+01 2.220273739D-03-1.964219980D-07
 9.262295070D-12-1.560026961D-16              -2.489244513D+05 1.263946278D+02
CL              Hf:CODATA1989.Spec:NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 7/97 CL  1.00    0.00    0.00    0.00    0.00 0   35.4527000     121301.000
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   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6271.588
 2.276215854D+04-2.168413293D+02 2.745185115D+00 2.451101694D-03-5.458011990D-06
 4.417986880D-09-1.288134004D-12                1.501357068D+04 3.102950764D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6271.588
-1.697932930D+05 6.081726460D+02 2.128664090D+00 1.307367034D-04-2.644883596D-08
 2.842504775D-12-1.252911731D-16                9.934387400D+03 8.844759410D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6271.588
-7.139687070D+07 4.499936330D+04-9.264315350D+00 1.657437964D-03-1.326219399D-07
 5.533998870D-12-8.390301878D-17               -3.405333030D+05 1.069111299D+02
CL+             Spec: NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 1/98 CL  1.00E  -1.00    0.00    0.00    0.00 0   35.4521514    1378799.635
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6386.335
 1.034697859D+05-1.293758873D+03 8.186702690D+00-9.916014600D-03 9.208472370D-06
-4.507426240D-09 9.182127880D-13                1.714758780D+05-2.766419200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6386.335
 4.056409480D+04-4.960165720D+01 3.101653630D+00-5.868738290D-04 2.252039316D-07
-3.299703020D-11 1.708780842D-15                1.652982337D+05 2.574929905D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6386.335
-3.078099946D+06-6.858418280D+02 3.092289282D+00-1.922260015D-05 3.805551560D-10
-1.571848967D-13 8.442513880D-18                1.683434405D+05 1.334394541D+00
CL-             JPCRD v14 n3 1985 p731.
 3 g 4/97 CL  1.00E   1.00    0.00    0.00    0.00 0   35.4532486    -233957.972
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.888389093D+04 4.200629330D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.888389093D+04 4.200629330D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.888389093D+04 4.200629330D+00
CLCN            TPIS 1991 v2 pt1 p230; pt2 p218
 2 g 6/95 CL  1.00C   1.00N   1.00    0.00    0.00 0   61.4701400     134200.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10669.042
 7.274043430D+04-1.297344947D+03 1.107676527D+01-1.108430216D-02 1.614009477D-05
-1.088916772D-08 2.830952246D-12 0.000000000D+00 2.084388986D+04-3.597370680D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10669.042
 3.467573120D+05-1.957857370D+03 8.807806150D+00-4.388362780D-04 1.024761895D-07
-1.110675026D-11 4.986179420D-16 0.000000000D+00 2.581923944D+04-2.636885997D+01
CLF             TPIS 1989 v1 pt1 p190; pt2 p97.
 2 tpis89 CL  1.00F   1.00    0.00    0.00    0.00 0   54.4511032     -55700.993
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8908.107
 3.352210810D+04-3.688311900D+02 4.272288620D+00 2.549434508D-03-4.456830890D-06
 3.413854120D-09-9.838685200D-13               -5.839369690D+03 2.317931556D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8908.107
 3.045867173D+06-9.979328260D+03 1.684162254D+01-7.465850620D-03 2.336213612D-06
-3.365865460D-10 1.763082415D-14                5.447120800D+04-8.707987920D+01
CLF3            TPIS 1989 v1 pt1 p193; pt2 p98.
 2 tpis89 CL  1.00F   3.00    0.00    0.00    0.00 0   92.4479096    -164600.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13728.449
 1.285175171D+05-2.140445721D+03 1.493096474D+01-6.042471040D-03 3.718968610D-06
-8.053201100D-10-7.985600530D-14               -1.138459640D+04-5.594838840D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13728.449
-2.294956235D+05-1.220741000D+02 1.009124644D+01-3.649724750D-05 8.058910750D-09
-9.230849950D-13 4.272569490D-17               -2.282840447D+04-2.511605966D+01
CLF5            TPIS 1989 v1 pt1 p194; pt2 p99.
 2 tpis89 CL  1.00F   5.00    0.00    0.00    0.00 0  130.4447160    -238000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17930.396
 2.459689770D+05-4.315332140D+03 2.726999940D+01-1.670185730D-02 1.421669140D-05
-6.426578480D-09 1.183153940D-12               -1.071431830D+04-1.267463220D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17930.396
-4.269366970D+05-2.057840510D+02 1.615461620D+01-6.210011950D-05 1.375710540D-08
-1.579849130D-12 7.327537460D-17               -3.361479390D+04-5.757506560D+01
CLO             TPIS 1989 v1 pt1 p180; pt2 p90.
 2 tpis89 CL  1.00O   1.00    0.00    0.00    0.00 0   51.4521000     101621.115
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9522.115
-1.687268145D+04 2.573812247D+02 2.175846120D+00 6.432061130D-03-8.568249500D-06
 5.764971250D-09-1.545771209D-12                9.829518980D+03 1.386009628D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9522.115
 4.093760520D+05-1.765985112D+03 7.087900630D+00-1.828450169D-03 7.103818100D-07
-1.209332942D-10 7.076441040D-15                2.151891784D+04-1.668646423D+01
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CLO2            TPIS v1 pt1 1989 p182; pt2 p91.
 2 g 7/93 CL  1.00O   2.00    0.00    0.00    0.00 0   67.4515000     105000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10800.646
-1.127277696D+04 3.903032030D+02-3.843018530D-01 2.108677947D-02-2.793137755D-05
 1.841289286D-08-4.839779150D-12 0.000000000D+00 9.756933670D+03 2.913262033D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10800.646
-1.633793802D+05-3.161480670D+02 7.009787260D+00 2.837971144D-04-1.179925338D-07
 2.920383252D-11-2.024030202D-15 0.000000000D+00 1.184946452D+04-1.091169494D+01
CL2             Chlorine gas. TPIS 1989, v1, pt2, p88.
 2 tpis89 CL  2.00    0.00    0.00    0.00    0.00 0   70.9054000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9181.110
 3.462817240D+04-5.547129490D+02 6.207591030D+00-2.989636730D-03 3.173034160D-06
-1.793634670D-09 4.260058630D-13                1.534070750D+03-9.438353030D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9181.110
 6.092566750D+06-1.949626880D+04 2.854534910D+01-1.449968280D-02 4.463889430D-06
-6.358524030D-10 3.327359310D-14                1.212117220D+05-1.690778320D+02
CL2O            TPIS 1989 v1 pt1 p184; pt2 p92.
 2 tpis89 CL  2.00O   1.00    0.00    0.00    0.00 0   86.9048000      79000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11695.482
 7.798855400D+04-1.182537879D+03 9.526514660D+00-2.596163176D-03 8.696781310D-07
 4.484098270D-10-3.044511967D-13                1.376729572D+04-2.484691754D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11695.482
-1.271743461D+05-6.741963220D+01 7.050022450D+00-1.988084386D-05 4.366209050D-09
-4.978580680D-13 2.295679186D-17                7.387289300D+03-8.797487610D+00
Co              Hf:Hultgren 1973 p128. Levels:JPCRD v14 sup2 1985 p513.
 3 g 7/97 CO  1.00    0.00    0.00    0.00    0.00 0   58.9332000     428441.600
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6359.768
-2.598939184D+03 2.461989844D+02-6.106058370D-01 1.393005772D-02-2.210012979D-05
 1.623755261D-08-4.534904351D-12                4.984613760D+04 2.257584199D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6359.768
 1.381841305D+06-3.756036680D+03 6.657130650D+00-1.269246675D-03 1.464092329D-07
 6.574946570D-12-1.102384178D-15                7.494442910D+04-2.258500836D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6359.768
-5.468015750D+08 4.037704950D+05-1.142413163D+02 1.663014422D-02-1.156228007D-06
 3.862515150D-11-5.002032746D-16               -3.076031798D+06 1.003028648D+03
Co+             JPCRD v14 sup2 1985.
 3 g 7/97 CO  1.00E  -1.00    0.00    0.00    0.00 0   58.9326514    1193003.307
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6291.507
 1.028494160D+05-8.744731260D+02 4.279500280D+00 2.225857835D-03-7.457274570D-06
 7.279221950D-09-2.347541963D-12                1.474895959D+05-5.679019220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6291.507
 2.907386174D+06-8.619705750D+03 1.188134934D+01-3.510647420D-03 5.748004680D-07
-2.534065135D-11 2.976607469D-16                1.977419221D+05-6.096533440D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6291.507
 2.701785479D+09-1.604232092D+06 3.687314770D+02-4.041150820D-02 2.371848586D-06
-7.119952160D-11 8.635423717D-16                1.293631390D+07-3.201662470D+03
Co-             JPCRD v14 n3 1985 p731.
 3 g 9/97 CO  1.00E   1.00    0.00    0.00    0.00 0   58.9337486     358414.372
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6306.772
 3.459493760D+04-1.355041712D+02 1.116330898D+00 9.042761830D-03-1.454296726D-05
 9.994940630D-09-2.595633259D-12                4.337037820D+04 1.270494975D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6306.772
-5.741394170D+05 1.763109207D+03 1.415561988D+00 3.776869690D-04-7.534179980D-08
 7.995701540D-12-3.490440000D-16                3.083493114D+04 1.634360353D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6306.772
-7.121795840D+05 7.962447120D+02 2.328870839D+00 1.919463732D-05-1.179708474D-09
 3.764228600D-14-4.875340940D-19                3.689285080D+04 9.511282720D+00
Cr              Hf:JANAF 6/79. Spec:JPCRD v14 sup2 1985 p264.
 3 g 7/97 CR  1.00    0.00    0.00    0.00    0.00 0   51.9961000     397480.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 1.335658217D+03-2.102424026D+01 2.631908173D+00-4.246263250D-04 7.439194160D-07
-6.763931630D-10 2.507855625D-13                4.715866640D+04 6.005425450D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.120220789D+07 3.401163690D+04-3.657062170D+01 2.110296902D-02-5.518180140D-06
 7.173601710D-10-3.505127367D-14               -1.688993440D+05 2.864481267D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 3.900886930D+09-2.462918543D+06 5.915632640D+02-6.697121640D-02 3.946957790D-06
-1.166504597D-10 1.367279456D-15                1.955381984D+07-5.133510550D+03
Cr+             Spec:JPCRD v14 sup2 1985.
 3 g 7/97 CR  1.00E  -1.00    0.00    0.00    0.00 0   51.9955514    1056546.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
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 1.819187467D+02-2.188843517D+00 2.510676511D+00-2.706791825D-05 3.768492630D-08
-2.736784742D-11 8.115389932D-15                1.263380825D+05 6.506276170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.342330790D+06-1.064261051D+04 1.557884307D+01-7.708971480D-03 2.158300274D-06
-2.368108110D-10 8.952805604D-15                1.932997670D+05-8.604356670D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.853867040D+08-4.114535830D+05 1.242898882D+02-1.610102894D-02 1.147677369D-06
-4.099673600D-11 5.728606039D-16                3.281645810D+06-1.034723629D+03
Cr-            JPCRD v14 n3 1985 p731.
 3 g10/97 CR  1.00E   1.00    0.00    0.00    0.00 0   51.9966486     327023.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.858627870D+04 6.566835370D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.858627870D+04 6.566835370D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.858627870D+04 6.566835370D+00
CrN
 2 J12/73 CR  1.00N   1.00    0.00    0.00    0.00 0   66.0028400     505021.510
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.930463600D+00 3.037704200D-03-1.271396400D-06
-1.178124900D-09 8.555134900D-13                5.974420300D+04 1.019188120D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.864960200D+00 8.516045600D-04-4.407075800D-07
 1.066760100D-10-8.373142200D-15                5.947743700D+04 5.295067570D+00
CrO
 2 J12/73 CR  1.00O   1.00    0.00    0.00    0.00 0   67.9955000     188285.447
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.841499600D+00 4.095335800D-03-3.577646300D-06
 8.171043900D-10 2.407200900D-13                2.164606700D+04 1.151799220D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.013981800D+00 6.270024500D-04-2.795679400D-07
 6.000310000D-11-4.405791600D-15                2.134669300D+04 5.551715100D+00
CrO2
 2 J12/73 CR  1.00O   2.00    0.00    0.00    0.00 0   83.9949000     -75312.810
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.301264500D+00 8.162585700D-03-5.890768000D-06
 1.617085600D-11 1.081626700D-12               -1.035356900D+04 1.139911380D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.849999800D+00 1.272510100D-03-5.492054800D-07
 1.049749100D-10-7.399548600D-15               -1.104218300D+04-1.744976320D+00
CrO3
 2 J12/73 CR  1.00O   3.00    0.00    0.00    0.00 0   99.9943000    -292879.663
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.907285800D+00 2.304960800D-02-2.650129400D-05
 1.286241300D-08-1.838199100D-12               -3.660868000D+04 1.534514150D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.162894600D+00 2.045083900D-03-8.859413100D-07
 1.697628200D-10-1.198776500D-14               -3.809255700D+04-1.589589450D+01
Cs             Hf:CODATA1989.Spec:NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 7/97 CS  1.00    0.00    0.00    0.00    0.00 0  132.9054500      76500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.466584070D+01-8.279346040D-01 2.504942210D+00-1.494620690D-05 2.425976774D-08
-2.013172322D-11 6.704271991D-15                8.459321390D+03 6.848825772D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 6.166040900D+06-1.896175522D+04 2.483229903D+01-1.251977234D-02 3.309017390D-06
-3.354012020D-10 9.626500908D-15                1.285111231D+05-1.522942188D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-9.566231720D+08 4.321690420D+05-6.371801020D+01 5.246260580D-03-2.366560159D-07
 5.848488480D-12-6.169370441D-17               -3.585268840D+06 6.156618174D+02
Cs+            Spec:NSRDS-NBS 35 v3 1971 p128.
 3 g 1/98 CS  1.00E  -1.00    0.00    0.00    0.00 0  132.9049014     458401.828
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                5.438737820D+04 6.182757992D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                5.438737820D+04 6.182757992D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
```

```
-2.479469300D+08 1.405115456D+05-2.805027359D+01 3.087928133D-03-1.273598265D-07
-3.748818380D-13 1.214944533D-16              -1.072498017D+06 2.756827325D+02
Cs-            JPCRD v14 n3 1985 p731.
 3 g10/97 CS  1.00E   1.00    0.00    0.00    0.00 0  132.9059986      24797.228
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.237029001D+03 6.182770382D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.237029001D+03 6.182770382D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.237029001D+03 6.182770382D+00
CsCL
 2 J 6/68 CS  1.00CL  1.00    0.00    0.00    0.00 0  168.3581500    -240166.789
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.182303000D+00 1.375955300D-03-2.058693300D-06
 1.483647400D-09-3.976454600D-13              -3.017792700D+04 6.638488236D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.479845500D+00 1.094916400D-04-3.998991400D-09
 2.064199500D-13 2.218464000D-17              -3.023580900D+04 5.217317436D+00
CsF
 2 J 6/68 CS  1.00F   1.00    0.00    0.00    0.00 0  151.9038532    -356483.908
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.744987900D+00 3.010051600D-03-4.588381600D-06
 3.217969400D-09-8.378601700D-13              -4.409069600D+04 7.194873545D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.437330900D+00 1.271500000D-04-2.054765000D-08
 2.981335700D-12-1.477424500D-16              -4.422799500D+04 3.873556245D+00
CsO
 2 J12/68 CS  1.00O   1.00    0.00    0.00    0.00 0  148.9048500      62763.052
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.985741900D+00 2.127925100D-03-3.217025500D-06
 2.276429500D-09-5.972197600D-13               6.289894000D+03 7.516022992D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.466028200D+00 1.156323200D-04-5.998918700D-09
 1.317669900D-13 5.763974500D-17               6.195030900D+03 5.214549092D+00
CsOH           JPCRD v26 n4 1997 p1031.
 2 g 9/97 CS  1.00O   1.00H   1.00    0.00    0.00 0  149.9127900    -256000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11834.689
 9.386960790D+03-5.009354260D+02 8.301351980D+00-3.235596840D-03 2.612406777D-06
-4.950613410D-10-1.038364927D-13              -3.025722427D+04-1.742194837D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11834.689
 8.967171130D+05-2.323978587D+03 7.959644870D+00 1.101149275D-04-6.466013970D-08
 1.045968201D-11-5.822514170D-16              -1.736258234D+04-1.864239624D+01
CsOH+
 2 J12/71 CS  1.00O   1.00H   1.00E  -1.00    0.00 0  149.9122414     443519.618
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.848715800D+00 6.890834600D-03-1.183932800D-05
 9.433537200D-09-2.722268500D-12               5.167816700D+04 3.084848910D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.729256300D+00 1.157132400D-03-3.104443100D-07
 3.709629100D-11-1.550946300D-15               5.162648300D+04-5.764818178D-01
Cs2
 2 J12/83 CS  2.00    0.00    0.00    0.00    0.00 0  265.8109000     107377.133
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.745882250D+00-2.638628190D-03 1.141393050D-05
-1.604305000D-08 6.561122940D-12               1.154448560D+04 7.606793172D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.866451780D+00-3.990143260D-03 1.319480840D-06
-1.634131860D-10 6.881259080D-15               1.080542930D+04-4.297494198D+00
Cs2CL2
 2 J 6/68 CS  2.00CL  2.00    0.00    0.00    0.00 0  336.7163000    -659831.356
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.295264200D+00 2.850560000D-03-4.557601900D-06
 3.255773100D-09-8.606736200D-13              -8.222286200D+04-7.518352964D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.942437500D+00 6.265930300D-05-2.633109700D-08
 4.891214200D-12-3.355415200D-16              -8.234585500D+04-1.059806004D+01
Cs2F2
 2 J 6/68 CS  2.00F   2.00    0.00    0.00    0.00 0  303.8077064    -890123.055
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   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.442556100D+00 6.492100100D-03-1.083275700D-05
 8.179105400D-09-2.317397800D-12              -1.097816500D+05-7.248244455D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.879372500D+00 1.267482900D-04-5.090525300D-08
 8.971176200D-12-5.809096000D-16              -1.100505700D+05-1.405482130D+01
Cs2O
 2 J12/68 CS  2.00O   1.00    0.00    0.00    0.00 0  281.8103000    -92046.757
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.755363900D+00 4.911607300D-03-7.707251800D-06
 5.415695700D-09-1.408089800D-12              -1.294682900D+04 4.300155036D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.897946700D+00 1.016509800D-04-3.806206200D-08
 6.146639300D-12-3.575821600D-16              -1.316998900D+04-1.165916464D+00
Cs2O2H2          JPCRD v26 n4 1997 p1031.
 2 g 9/97 CS  2.00O   2.00H   2.00    0.00    0.00 0  299.8255800    -653000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23937.353
-1.085981041D+04-6.883068420D+02 1.643543354D+01-4.039220580D-03 2.331117156D-06
 8.439651630D-10-6.859309730D-13              -7.939476230D+04-4.906196810D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23937.353
 1.802857941D+06-4.656354750D+03 1.693566597D+01 2.117402535D-04-1.272249096D-07
 2.066555839D-11-1.152390667D-15              -5.190813690D+04-5.849719160D+01
Cs2SO4
 2 J 6/79 CS  2.00S   1.00O   4.00    0.00    0.00 0  361.8745000   -1122581.398
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.296538500D+00 4.485430000D-02-6.098792300D-05
 4.051638800D-08-1.067349500D-11              -1.378255900D+05 1.340963744D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.541904500D+01 4.052765000D-03-1.791034100D-06
 3.502465300D-10-2.521573600D-14              -1.403677500D+05-4.149218456D+01
Cu               Hf:CODATA,1989. Spec:JPCRD v19 n3 1990.
 3 g12/97 CU  1.00    0.00    0.00    0.00    0.00 0   63.5460000    337400.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 7.713133150D+01-1.169236206D+00 2.506987803D+00-2.116434879D-05 3.441714710D-08
-2.862608999D-11 9.559250991D-15              3.983981210D+04 5.730813220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 2.308090411D+06-8.503261000D+03 1.467859102D+01-8.467136520D-03 2.887821016D-06
-4.270659180D-10 2.304265084D-14              9.207535620D+04-7.854701560D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
-6.490595890D+08 4.240323360D+05-1.028965806D+02 1.297259934D-02-7.766697680D-07
 2.220446727D-11-2.441532031D-16              -3.305304580D+06 9.198622920D+02
Cu+              JPCRD v19 n3 1990 p527.
 3 g 6/97 CU  1.00E  -1.00    0.00    0.00    0.00 0   63.5454514   1089079.728
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 4.170301540D-04-5.724434000D-06 2.500000032D+00-9.363351990D-11 1.485217665D-13
-1.197844347D-16 3.853191729D-20              1.302400623D+05 5.075939950D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
-2.181443045D+06 7.217858160D+03-6.941154650D+00 6.208248860D-03-2.139340484D-06
 3.566431430D-10-2.081198499D-14              8.516456670D+04 7.116800600D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 2.994686622D+09-1.831416153D+06 4.294927050D+02-4.801927810D-02 2.836504302D-06
-8.452189210D-11 1.013018232D-15              1.468809300D+07-3.729918090D+03
Cu-              JPCRD v14 n3 1985 p731.
 3 g10/97 CU  1.00E   1.00    0.00    0.00    0.00 0   63.5465486    212718.628
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              2.483864954D+04 5.075966030D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              2.483864954D+04 5.075966030D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              2.483864954D+04 5.075966030D+00
CuCL
 2 J 3/66 CU  1.00CL  1.00    0.00    0.00    0.00 0   98.9987000     91088.442
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.349160000D+00 5.102830200D-03-9.127800200D-06
 7.601415500D-09-2.398448900D-12              9.796756200D+03 8.269473040D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.390298800D+00 1.834948400D-04-5.711070300D-08
 1.129332100D-11-8.197552000D-16              9.609726600D+03 3.392165140D+00
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CuF
 2 J12/77 CU  1.00F   1.00    0.00    0.00    0.00 0   82.5444032    -12552.131
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.765450500D+00 6.851180500D-03-1.133881900D-05
 8.909657800D-09-2.692769200D-12              -2.554856500D+03 9.872774110D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.122739900D+00 6.316346300D-04-3.347282000D-07
 8.083736700D-11-5.783481700D-15              -2.800595300D+03 3.485645710D+00
CuF2
 2 J12/77 CU  1.00F   2.00    0.00    0.00    0.00 0  101.5428064    -266945.896
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.110769600D+00 1.432580700D-02-2.281174300D-05
 1.727889300D-08-5.072697700D-12              -3.350045300D+04 1.099956980D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.818423600D+00-1.649790800D-04 2.029177400D-07
-2.545311300D-11 1.206573200D-16              -3.432274400D+04-7.128629210D+00
CuO
 2 J12/77 CU  1.00O   1.00    0.00    0.00    0.00 0   79.5454000    306276.724
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.709352000D+00 3.196505900D-03-5.297010900D-06
 4.216423800D-09-1.289185500D-12               3.562747000D+04 6.331400790D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.272362500D+00 4.471327600D-04-2.395697900D-07
 6.040531600D-11-4.245601600D-15               3.553534900D+04 3.727018890D+00
Cu2
 2 J 9/66 CU  2.00    0.00    0.00    0.00    0.00 0  127.0920000    485356.654
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.924435800D+00 2.727494900D-03-4.919495600D-06
 4.182196500D-09-1.339353300D-12               5.711918700D+04 6.083808290D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.423973400D+00 2.024895200D-04-6.448979300D-08
 1.406541200D-11-7.602049400D-16               5.703813100D+04 3.785355790D+00
Cu3CL3
 2 J 3/66 CU  3.00CL  3.00    0.00    0.00    0.00 0  296.9961000    -258575.302
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.144290000D+01 2.069080600D-02-3.826400300D-05
 3.234105300D-08-1.030988400D-11              -3.515161000D+04-1.826878650D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.562612700D+01 4.337383300D-04-1.946700600D-07
 3.846693800D-11-2.789970000D-15              -3.588185300D+04-3.775233450D+01
D              D0(D2):JMolSpc,v33 1970 p147. NSRDS-NBS 3 SEC 6 1972.
 3 g 6/97 D   1.00    0.00    0.00    0.00    0.00 0    2.0141020    221720.228
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              2.592128700D+04 5.917143380D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 6.050019210D+01-1.810766064D-01 2.500210817D+00-1.220711706D-07 3.715172170D-11
-5.660680210D-15 3.393920393D-19              2.592243752D+04 5.902125370D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.169259778D+08-1.309309862D+05 3.392595050D+01-3.805973810D-03 2.427699393D-07
-7.677967800D-12 9.624191177D-17              1.065922040D+06-2.726201602D+02
D+             CP/R=2.5. IP for D: Moore NSRDS-NBS 3 SEC 6 1972.
 3 g 9/96 D   1.00E  -1.00    0.00    0.00    0.00 0    2.0135534    1540324.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              1.845120037D+05-1.018414521D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              1.845120037D+05-1.018414521D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              1.845120037D+05-1.018414521D-01
D-             JPCRD v14 n3 1985 p731.
 3 g/8/96 D   1.00E   1.00    0.00    0.00    0.00 0    2.0146506    142752.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              1.642373393D+04-1.010243437D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              1.642373393D+04-1.010243437D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
```

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 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.642373393D+04-1.010243437D-01
DBr             TPIS, vol 1 part 1,1989 p.206-207 AND part 2 p.107.
 2 tpis89 D   1.00BR  1.00    0.00    0.00    0.00 0   81.9181020     -37036.447
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8668.104
-1.945076370D+04 2.058144800D+02 3.023812300D+00-1.431428680D-03 6.789351620D-06
-6.532109890D-09 2.076823010D-12                -6.578303780D+03 8.124745900D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8668.104
 6.652417580D+05-2.593701890D+03 6.885511060D+00-1.103111670D-03 2.893770800D-07
-3.151499220D-11 1.010745160D-15                1.037557730D+04-1.973433580D+01
DCL             TPIS, vol 1 part 1,1989 p.188-89 AND part 2 p.95.
 2 tpis89 D   1.00CL  1.00    0.00    0.00    0.00 0   37.4668020     -93547.003
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8661.104
 1.046420900D+04-2.313813250D+02 5.420693150D+00-7.508012340D-03 1.398672450D-05
-1.066249530D-08 3.011167540D-12                -1.128403380D+04-6.711853750D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8661.104
 4.117283350D+05-1.764534910D+03 5.668876800D+00-3.475962790D-04 5.882684600D-08
 3.760295980D-13-5.164602680D-16                -1.541260140D+03-1.275660390D+01
DF              TPIS, vol 1, part 1,1989 p.172-73, part 2, p.80-81.
 3 tpis89 D   1.00F   1.00    0.00    0.00    0.00 0   21.0125052    -276227.001
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8638.104
 5.721310920D+04-7.311665600D+02 7.220839690D+00-9.423896160D-03 1.208015820D-05
-6.941751490D-09 1.538509260D-12                -3.069226270D+04-1.932743100D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8638.104
 8.001155020D+05-2.438382430D+03 5.620660280D+00-2.020397160D-04 1.714369970D-08
 2.697524030D-12-2.888327920D-16                -1.857442760D+04-1.473001390D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8638.104
 5.971823870D+07-8.331260740D+04 3.456042390D+01-4.650865170D-03 3.665717550D-07
-1.411792640D-11 2.114290770D-16                5.807634280D+05-2.577007690D+02
DOCL
 2 J 3/79 D   1.00O   1.00CL  1.00    0.00    0.00 0   53.4662020     -78243.308
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.479041800D+00 1.084589600D-02-1.522830500D-05
 1.143731400D-08-3.420492500D-12                -1.051809200D+04 1.212671070D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.435076100D+00 2.532238700D-03-1.031233100D-06
 1.900545400D-10-1.268238400D-14                -1.091940200D+04 2.727159690D+00
DO2             TPIS 1989 v1 pt1 p138; pt2 p49.
 2 tpis89 D   1.00O   2.00    0.00    0.00    0.00 0    34.01290       6487.344
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10065.344
-2.111479735D+04 6.023371750D+02-1.294877674D+00 1.812947970D-02-2.161807666D-05
 1.391729127D-08-3.697740280D-12 0.000000000D+00-2.976943856D+03 3.272834480D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10065.344
-1.267224927D+06 2.799947016D+03 2.325174609D+00 2.726325070D-03-6.314507320D-07
 6.729289200D-11-2.765192818D-15 0.000000000D+00-1.959411733D+04 1.789922833D+01
DO2-            TPIS 1989 v1 pt1 p139; pt2 p50.
 2 tpis89 D   1.00O   2.00E   1.00    0.00    0.00 0    34.01345    -104795.510
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10079.890
 1.048705051D+05-8.906236770D+02 5.666553560D+00 1.904603784D-03-1.215263210D-06
 6.577513330D-10-2.147376147D-13 0.000000000D+00-8.942377250D+03-7.797219200D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10079.890
 5.527661920D+05-2.796895783D+03 8.772206670D+00-6.291116630D-04 1.272331622D-07
-1.364440687D-11 6.005199440D-16 0.000000000D+00 2.512066767D+03-2.890020381D+01
D2              Deuterium. TPIS, 1989, v1, pt2, pp45-6.
 3 tpis89 D   2.00    0.00    0.00    0.00    0.00 0    4.0282040         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8569.103
 2.125789890D+04-2.996945070D+02 5.130314510D+00-4.172969580D-03 5.014343800D-06
-2.126388540D-09 2.386532770D-13                3.944981900D+02-1.164190950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8569.103
 8.215156410D+05-2.365619830D+03 5.342971060D+00 6.928322170D-05-8.523717940D-08
 2.456453640D-11-1.960600940D-15                1.434212440D+04-1.712597860D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8569.103
 4.899684730D+08-3.112796170D+05 7.945732020D+01-8.425549490D-03 4.789273710D-07
-1.390855370D-11 1.637521280D-16                2.460031030D+06-6.636810040D+02
D2+
 2 J 9/77 D   2.00E  -1.00    0.00    0.00    0.00 0    4.0276554    1498605.661
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.807514000D+00-3.110626000D-03 1.016298200D-05
-9.836327100D-09 3.265985300D-12                1.791709600D+05-2.286628250D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.589180000D+00 8.921465100D-04-2.426448400D-07
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 5.758440900D-11-6.738056000D-15                1.790375200D+05-2.058178850D+00
D2-
 2 J 9/77 D   2.00E   1.00    0.00    0.00    0.00 0    4.0287526     235371.941
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.214480000D+00 7.835816500D-04 3.589268500D-06
-5.239419000D-09 2.087136500D-12                2.729300900D+04 3.681558370D-01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.753104200D+00 9.801899100D-04-3.638796000D-07
 7.070048200D-11-5.067427200D-15                2.706470800D+04-2.819551720D+00
D2O             TPIS 1989 v1 pt1 p142; pt2 p51.
 2 g 6/99 D   2.00O   1.00    0.00    0.00    0.00 0   20.0276040    -249210.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9960.017
 6.958278470D+03-1.280889437D+01 3.595878870D+00 1.502093683D-03 3.594675050D-07
 5.340417200D-10-5.181941270D-13 0.000000000D+00-3.101944566D+04 2.895556576D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9960.017
 1.544193253D+06-5.474238900D+03 1.017542424D+01-9.619415540D-04 2.036545675D-07
-2.050566442D-11 8.510770690D-16 0.000000000D+00 2.983248980D+03-4.465011570D+01
D2O2            TPIS 1989 v1 pt1 p142; pt2 p52.
 2 g 6/99 D   2.00O   2.00    0.00    0.00    0.00 0   36.0270040    -144300.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11565.639
 2.957711324D+04-6.893037570D+01 2.043905473D+00 1.570281822D-02-1.935478714D-05
 1.384941336D-08-4.104184900D-12 0.000000000D+00-1.802502679D+04 1.347156482D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11565.639
 1.147867936D+06-5.225760930D+03 1.311088701D+01-1.179811896D-03 2.729336904D-07
-2.961433535D-11 1.310306129D-15 0.000000000D+00 1.219580532D+04-5.690538200D+01
D2S
 2 J 6/77 D   2.00S   1.00    0.00    0.00    0.00 0   36.0942040     -23890.981
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.807082400D+00 3.759631100D-04 5.753079900D-06
-5.348574000D-09 1.405408300D-12               -4.066121900D+03 3.879287490D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.666290100D+00 3.499226400D-03-1.420728400D-06
 2.668563900D-10-1.868473900D-14               -4.214730800D+03 3.799699690D+00
F               Hf:CODATA1989. NSRDS-NBS 35 1971 & 34 1970.
 3 g 5/97 F   1.00    0.00    0.00    0.00    0.00 0   18.9984032      79380.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6518.460
 1.137409088D+03-1.453392797D+02 4.077403610D+00-4.303360140D-03 5.728897740D-06
-3.819312900D-09 1.018322509D-12                9.311110120D+03-3.558982650D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6518.460
 1.473506226D+04 8.149927360D+01 2.444371819D+00 2.120210026D-05-4.546918620D-09
 5.109528730D-13-2.333894647D-17                8.388374650D+03 5.478710640D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6518.460
-2.926724756D+07 1.775674924D+04-1.814463258D+00 5.351200280D-04-3.513620800D-08
 1.101519690D-12-1.061293837D-17               -1.319642721D+05 4.248814560D+01
F+              Moore: NSRDS-NBS 35 1971 p62; NSRDS-NBS 34 1970 p6a.
 3 g 3/97 F   1.00E  -1.00    0.00    0.00    0.00 0   18.9978546    1766816.332
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6710.732
-3.871680190D+04 3.218815660D+02 2.200920452D+00-2.455492688D-04 7.858355060D-07
-6.435987920D-10 1.839793564D-13                2.098830937D+05 7.816999240D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6710.732
 1.649635664D+04 1.337351478D+02 2.332522942D+00 1.215277877D-04-4.801037700D-08
 9.027225150D-12-5.470664940D-16                2.110745327D+05 6.625817090D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6710.732
 7.599619330D+06-1.391106563D+03 1.714871534D+00 2.428311844D-04-1.894860146D-08
 6.420828070D-13-8.257979730D-18                2.269126001D+05 1.102848944D+01
F-              JPCRD v14 n3 1985 p731.
 3 g 1/98 F   1.00E   1.00    0.00    0.00    0.00 0   18.9989518    -255092.072
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.142572443D+04 3.264882710D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.142572443D+04 3.264882710D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.142572443D+04 3.264882710D+00
FCN             TPIS 1991 v2 pt1 p229; pt2 p217.
 2 g 5/99 F   1.00C   1.00N   1.00    0.00    0.00 0   45.0158432      34327.854
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10128.960
 3.984454120D+04-6.988655360D+02 7.058839660D+00-1.404863382D-03 3.964652510D-06
-3.045609294D-09 7.923045900D-13 0.000000000D+00 6.172627570D+03-1.505643041D+01
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   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10128.960
 3.981873550D+05-2.302971079D+03 9.027081390D+00-5.228710260D-04 1.191059272D-07
-1.280287231D-11 5.733807190D-16 0.000000000D+00 1.588449451D+04-2.984971849D+01
FO              Chase 1996 JPCRD v25 n2 p551.
 2 j 9/95 F   1.00O   1.00    0.00    0.00    0.00 0   34.9978032     109012.100
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9388.000
-3.912182440D+04 7.967036940D+02-1.634777767D+00 1.601810071D-02-2.095210771D-05
 1.382740666D-08-3.664524950D-12 0.000000000D+00 8.375525230D+03 3.383325720D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9388.000
-1.597940503D+06 4.377376380D+03-4.897507640D-01 2.682336321D-03-6.900804850D-07
 7.246479680D-11-2.726912632D-15 0.000000000D+00-1.644248211D+04 3.559923610D+01
FO2,FOO         Chase 1996 JPCRD v25 n2 p551.
 2 j 9/95 F   1.00O   2.00    0.00    0.00    0.00 0   50.9972032      25400.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11255.813
 5.819121260D+03-2.346897182D+02 5.437003700D+00 2.166959682D-03 3.654785760D-07
-2.070330854D-09 9.427716600D-13 0.000000000D+00 2.694645218D+03-1.166414457D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11255.813
-1.213177293D+06 2.493436116D+03 4.465038840D+00 9.416205510D-04-6.426686480D-08
-1.085619597D-11 1.216984745D-15 0.000000000D+00-1.596825164D+04 8.655417510D+00
FO2,OFO         Chase 1996 JPCRD v25 n2 p551.
 2 j 9/95 F   1.00O   2.00    0.00    0.00    0.00 0   50.9972032     378600.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10538.382
-7.734106400D+04 1.663800209D+03-9.612815160D+00 4.989156870D-02-6.946217130D-05
 4.707787800D-08-1.258890729D-11 0.000000000D+00 3.697092730D+04 7.795943040D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10538.382
-6.211867340D+05 9.369474590D+02 6.401558750D+00 2.136110846D-04-4.337977650D-08
 4.667312240D-12-2.059767432D-16 0.000000000D+00 3.638357270D+04-6.150264330D+00
F2              TPIS 1989. v1 pt2 p73.
 2 tpis89 F   2.00    0.00    0.00    0.00    0.00 0   37.9968064         0.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8825.106
 1.018176308D+04 2.274241183D+01 1.971353040D+00 8.151604010D-03-1.148960090D-05
 7.958652530D-09-2.167079526D-12              -9.586943000D+02 1.130600296D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8825.106
-2.941167790D+06 9.456597700D+03-7.738616150D+00 7.644712990D-03-2.241007605D-06
 2.915845236D-10-1.425033974D-14              -6.071005610D+04 8.423835080D+01
F2O             TPIS 1989 v1 pt1 p161; pt2 p76.
 2 g 4/99 F   2.00O   1.00    0.00    0.00    0.00 0   53.9962064      24500.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10911.521
 3.082919995D+04-2.299506259D+02 2.603805825D+00 1.586111264D-02-2.345633734D-05
 1.679619314D-08-4.703560330D-12 0.000000000D+00 3.055185332D+03 1.050933022D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10911.521
-1.885374518D+05-2.100729689D+02 7.151239160D+00 1.327687906D-04 1.804705706D-08
-1.416973671D-12 6.489389390D-17 0.000000000D+00 1.449129965D+03-1.257858336D+01
F2O2            FOOF. Chase 1996 JPCRD v25 n2 p551.
 2 j 9/95 F   2.00O   2.00    0.00    0.00    0.00 0   69.9956064      19200.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13778.453
 5.612270460D+04-9.985952230D+02 8.980649390D+00 6.421900870D-03-9.888516020D-06
 6.858061010D-09-1.842137493D-12 0.000000000D+00 5.298712590D+03-2.239292195D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13778.453
-2.190563532D+05-3.910920810D+02 1.029107144D+01-1.163345202D-04 2.570922521D-08
-2.949199983D-12 1.367386916D-16 0.000000000D+00 8.278020940D+02-2.756752555D+01
FS2F,fluorodisu   Difluorodisulfane. JPCRD 1985 sup1 v14 pt2 p1104.
 2 j 6/76 F   2.00S   2.00    0.00    0.00    0.00 0  102.1288064    -336435.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14595.300
 1.144462280D+05-1.853247564D+03 1.394098518D+01-4.043689370D-03 1.370970316D-06
 6.711903100D-10-4.624954960D-13 0.000000000D+00-3.351068330D+04-4.849212420D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14595.300
-2.077097921D+05-1.094539831D+02 1.008136946D+01-3.239537910D-05 7.125225270D-09
-8.134787410D-13 3.755022410D-17 0.000000000D+00-4.349446060D+04-2.346913121D+01
Fe              Cons:JPCRD v14 sup2 1985. Hf:Hultgren 1973.
 3 g 5/97 FE  1.00    0.00    0.00    0.00    0.00 0   55.8450000     415471.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6850.327
 6.790822660D+04-1.197218407D+03 9.843393310D+00-1.652324828D-02 1.917939959D-05
-1.149825371D-08 2.832773807D-12              5.466995940D+04-3.383946260D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6850.327
-1.954923682D+06 6.737161100D+03-5.486410970D+00 4.378803450D-03-1.116286672D-06
 1.544348856D-10-8.023578182D-15              7.137370060D+03 6.504979860D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6850.327
 1.216352511D+09-5.828563930D+05 9.789634510D+01-5.370704430D-03 3.192037920D-08
 6.267671430D-12-1.480574914D-16              4.847648290D+06-8.697289770D+02
Fe+             Spec:JPCRD v14 sup2 1985.
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 3 g 3/98 FE  1.00E  -1.00    0.00    0.00    0.00 0   55.8444514    1184217.849
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6935.749
-5.691231620D+04 1.847134390D+02 4.196972120D+00-5.978275970D-03 1.054267912D-05
-8.059804320D-09 2.256925874D-12                 1.401206571D+05-3.602542580D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6935.749
-8.176450090D+05 1.925359408D+03 1.717387154D+00 3.385338980D-04-9.813533120D-08
 2.228179208D-11-1.483964439D-15                 1.286352466D+05 1.500256262D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6935.749
 1.065217491D+08-2.883923997D+04-2.821752459D+00 2.712846797D-03-3.107069182D-07
 1.543726493D-11-2.725133516D-16                 4.142981690D+05 4.053497330D+01
Fe-            JPCRD v14 n3 1985 p731.
 3 g 9/97 FE  1.00E   1.00    0.00    0.00    0.00 0   55.8455486     393338.036
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6641.836
 1.341276767D+05-1.775438064D+03 1.084366935D+01-1.499440282D-02 1.412129744D-05
-6.942189050D-09 1.410953082D-12                 5.519472530D+04-4.140886490D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6641.836
-1.237808631D+05 8.249279070D+02 1.912936452D+00 2.280194065D-04-4.942014160D-08
 5.591493490D-12-2.566386941D-16                 4.156251610D+04 1.265367627D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6641.836
-1.008467687D+06 7.642402360D+02 2.332880311D+00 1.892649914D-05-1.170322571D-09
 3.749758920D-14-4.871021520D-19                 4.111417150D+04 9.680921840D+00
FeC5O5
 2 J 3/78 FE  1.00C   5.00O   5.00    0.00    0.00 0  195.8955000    -727858.869
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.606546000D+00 7.504212900D-02-1.220127500D-04
 1.005537800D-07-3.226097300D-11                -9.195143800D+04-2.576044492D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.116402100D+01 1.033310300D-02-4.331093600D-06
 8.204749700D-10-5.777387400D-14                -9.488893400D+04-7.207369028D+01
FeCL
 2 J 6/65 FE  1.00CL  1.00    0.00    0.00    0.00 0   91.2977000     251035.967
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.788582600D+00 4.367801100D-03-6.692232800D-06
 4.170745400D-09-8.468677300D-13                 2.892009700D+04 8.353334700D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.694066900D+00 1.160407800D-04-2.084017500D-08
-1.762655600D-12 5.231381400D-16                 2.879034400D+04 4.193522200D+00
FeCL2
 2 J12/70 FE  1.00CL  2.00    0.00    0.00    0.00 0  126.7504000    -140999.994
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.455750500D+00 7.963292700D-03-1.259396400D-05
 8.997673400D-09-2.324236300D-12                -1.884429700D+04 3.022818520D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.949260100D+00 5.337164100D-04 7.022120700D-08
-6.147549000D-11 6.793314300D-15                -1.904583200D+04-3.759538080D+00
FeCL3
 2 J 6/65 FE  1.00CL  3.00    0.00    0.00    0.00 0  162.2031000    -253119.989
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.561487300D+00 9.733824900D-03-1.554330500D-05
 1.118636800D-08-3.002299800D-12                -3.301362400D+04-3.985850530D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.777110600D+00 2.442136200D-04-1.031399400D-07
 1.920742600D-11-1.317929900D-15                -3.343957000D+04-1.454916480D+01
FeO
 2 J 9/66 FE  1.00O   1.00    0.00    0.00    0.00 0   71.8444000     251047.084
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.824525600D+00 4.304920700D-03-4.108478100D-06
 1.320118900D-09 7.131621700D-14                 2.919403500D+04 1.189113420D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.204981700D+00 2.683845200D-04-8.942673600D-08
 3.185591100D-11-3.392254300D-15                 2.882917000D+04 4.830389830D+00
Fe(OH)2
 2 J12/66 FE  1.00O   2.00H   2.00    0.00    0.00 0   89.8596800    -330536.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.676677340D+00 6.169314640D-02-1.207389950D-04
 1.098140260D-07-3.728568310D-11                -4.112897080D+04 2.967713760D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.962620120D+00 4.201373420D-03-1.610174430D-06
 2.683470760D-10-1.634973050D-14                -4.279943580D+04-1.869127010D+01
Fe2CL4
 2 J12/70 FE  2.00CL  4.00    0.00    0.00    0.00 0  253.5008000    -431373.784
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   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.273824200D+01 1.323555800D-02-2.164187300D-05
 1.599366700D-08-4.350709700D-12              -5.610657900D+04-1.982477280D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.535750000D+01 6.420786100D-04 2.081773000D-08
-5.158055900D-11 6.067349500D-15              -5.651003700D+04-3.189661080D+01
Fe2CL6
 2 J 6/65 FE  2.00CL  6.00    0.00    0.00    0.00 0  324.4062000    -654377.600
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.422118080D+01 4.354859680D-02-9.603901880D-05
 9.374630810D-08-3.360516260D-11              -8.419962650D+04-2.592448790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.156450310D+01 4.623490150D-04-1.849520780D-07
 3.201430430D-11-2.010027370D-15              -8.524323750D+04-5.865383700D+01
GaBr            Hf0,Props: TPIS 1996 pt1 p239, pt2 p193
 2 tpis96 GA  1.00BR  1.00    0.00    0.00    0.00 0  149.6270000    -17967.880
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9932.119
-2.185275415D+03-7.672232970D+01 4.770805670D+00-4.497881060D-04 5.579853600D-07
-3.065156457D-10 7.042946040D-14              -3.138004818D+03 2.948144294D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9932.119
 3.359805030D+05-8.406836680D+02 5.145084730D+00-3.265526000D-05-7.671022750D-08
 3.635123820D-11-3.358177830D-15               2.035179445D+03-4.277894080D-01
GaBr2           D0,cons: TPIS 1996 pt1 p241; pt2 p194.
 2 tpis96 GA  1.00BR  2.00    0.00    0.00    0.00 0  229.5310000    -149180.952
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14024.948
 7.081681620D+03-3.705766100D+02 8.418425360D+00-3.001930915D-03 3.595477670D-06
-2.276883735D-09 5.913221770D-13              -1.821116655D+04-9.512572050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14024.948
-3.302294360D+05 4.766722650D+02 7.104725400D+00-5.522771210D-04 3.159876015D-07
-5.513637150D-11 3.173293230D-15              -2.365683620D+04-1.162714892D+00
GaBr3           Subl,cons: TPIS 1996 pt1 p243; pt2 p196.
 2 tpis96 GA  1.00BR  3.00    0.00    0.00    0.00 0  309.4350000    -292962.663
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19037.337
 6.363807340D+03-5.142040450D+02 1.196065138D+01-4.134637650D-03 4.933978330D-06
-3.111868526D-09 8.043631480D-13              -3.570415500D+04-2.556896053D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19037.337
-5.103063750D+04-9.395209690D+00 1.000768765D+01-3.295954300D-06 7.679838140D-10
-9.175147260D-14 4.391186940D-18              -3.833402150D+04-1.410315914D+01
GaCL            Hf0,Props: TPIS 1996 pt1 p231, pt2 p186
 2 tpis96 GA  1.00CL  1.00    0.00    0.00    0.00 0  105.1757000    -69621.440
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9609.116
 6.417143000D+03-2.257949147D+02 5.311673690D+00-1.562280975D-03 1.836579731D-06
-1.100421873D-09 2.725812445D-13              -8.593892330D+03-1.695916014D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9609.116
-4.864842240D+05 1.452870183D+03 2.719542959D+00 1.144285628D-03-3.431452860D-07
 5.470440480D-11-3.019622103D-15              -1.895084035D+04 1.570925717D+01
GaCL2           D0,cons: TPIS 1996 pt1 p232; pt2 p187.
 2 tpis96 GA  1.00CL  2.00    0.00    0.00    0.00 0  140.6284000    -220978.909
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13513.391
 2.225481851D+04-6.046218440D+02 9.220388910D+00-4.554400790D-03 5.324855180D-06
-3.308605570D-09 8.462235560D-13              -2.564550386D+04-1.685409902D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13513.391
-3.445405300D+05 4.714437160D+02 7.108775480D+00-5.539433560D-04 3.163638240D-07
-5.518023930D-11 3.175353030D-15              -3.230936160D+04-3.744847140D+00
GaCL3           Subl,cons: TPIS 1996 pt1 p235; pt2 p189.
 2 tpis96 GA  1.00CL  3.00    0.00    0.00    0.00 0  176.0811000    -432624.753
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17375.247
 4.784948400D+04-1.162678125D+03 1.408954213D+01-8.106134290D-03 9.219430160D-06
-5.599710550D-09 1.404852600D-12              -4.915909730D+04-4.282180150D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17375.247
-9.466917310D+04-2.561468254D+01 1.002010048D+01-8.354073070D-06 1.901439055D-09
-2.231168493D-13 1.052949609D-17              -5.518201430D+04-1.864959150D+01
GaF             D0,Props: TPIS 1996 pt1 p224, pt2 p179
 2 tpis96 GA  1.00F   1.00    0.00    0.00    0.00 0   88.7214032    -232608.491
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9081.109
 3.670398010D+04-5.336572220D+02 5.759291920D+00-1.506128492D-03 9.509038450D-07
-1.830941130D-10-3.135959193D-14              -2.647075690D+04-6.589321880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9081.109
-2.983392279D+05 7.225157870D+02 3.639557430D+00 5.546736760D-04-1.464901450D-07
 2.177385396D-11-1.031058874D-15              -3.408528710D+04 7.553960000D+00
GaF2            D0,cons: TPIS 1996 pt1 p225; pt2 p180.
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 2 tpis96 GA  1.00F   2.00    0.00    0.00    0.00 0  107.7198064    -516712.441
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12115.659
 6.842539530D+04-8.897617740D+02 7.707455490D+00 2.072150890D-03-5.289981930D-06
 4.564127420D-09-1.406942753D-12               -5.919856150D+04-1.341142116D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12115.659
 4.100251360D+05-1.723259472D+03 8.951329220D+00-1.059205682D-03 2.745755154D-07
-2.907681311D-11 1.084834142D-15               -5.376571600D+04-2.113835528D+01
GaF3            Subl,cons: TPIS 1996 pt1 p226; pt2 p182.
 2 tpis96 GA  1.00F   3.00    0.00    0.00    0.00 0  126.7182096    -921476.983
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15223.017
 9.593266700D+04-1.355507494D+03 1.097760197D+01 3.461571720D-03-8.469551950D-06
 7.222468930D-09-2.213328653D-12               -1.061479087D+05-3.212651850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15223.017
-2.096961760D+05-1.431211274D+02 1.010568378D+01-4.184936820D-05 9.164759450D-09
-1.042661957D-12 4.799163450D-17               -1.136678134D+05-2.392539330D+01
GaH             D0,Props: TPIS 1996 pt1 p220, pt2 p177
 2 tpis96 GA  1.00H   1.00    0.00    0.00    0.00 0   70.7309400     214323.404
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8673.104
-4.391876200D+04 6.254457120D+02 3.276862890D-01 6.496641500D-03-3.802970010D-06
 2.852103704D-10 3.626809130D-13               2.171260108D+04 2.224032244D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8673.104
 3.257993990D+06-1.109099502D+04 1.801126796D+01-8.167719110D-03 2.601293566D-06
-3.813459350D-10 2.028049649D-14               9.369778240D+04-9.820900220D+01
GaI             Hf0,Props: TPIS 1996 pt1 p247, pt2 p200
 2 tpis96 GA  1.00I   1.00    0.00    0.00    0.00 0  196.6274700      44871.122
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10109.122
-3.661855030D+03-3.206924180D+01 4.599961920D+00-8.899475460D-05 1.162792633D-07
-1.812351457D-11-7.584619640D-15               4.198649370D+03 4.928964650D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10109.122
 1.498356654D+06-4.551967240D+03 9.803005350D+00-2.943735609D-03 8.658040510D-07
-1.106638204D-10 5.007836860D-15               3.291811910D+04-3.227359770D+01
GaI2            D0,cons: TPIS 1996 pt1 p249; pt2 p201.
 2 tpis96 GA  1.00I   2.00    0.00    0.00    0.00 0  323.5319400     -28954.965
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14470.935
-9.831395900D+02-2.152621259D+02 7.844318760D+00-1.819797849D-03 2.210706958D-06
-1.416110855D-09 3.713762930D-13               -4.534090230D+03-4.250516810D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14470.935
-3.202879750D+05 4.796502330D+02 7.102333960D+00-5.512657830D-04 3.157543452D-07
-5.510871940D-11 3.171977730D-15               -9.180919610D+03 7.275204880D-01
GaI3            Subl,cons: TPIS 1996 pt1 p250; pt2 p203.
 2 tpis96 GA  1.00I   3.00    0.00    0.00    0.00 0  450.4364100    -115877.240
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20122.760
-5.663472650D+03-2.425937116D+02 1.095451119D+01-2.059175489D-03 2.499117622D-06
-1.596502506D-09 4.167644060D-13               -1.576722832D+04-1.646129942D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20122.760
-3.164040130D+04-4.208662830D+00 1.000352001D+01-1.532650180D-06 3.611531540D-10
-4.350978870D-14 2.095704875D-18               -1.700058453D+04-1.090291552D+01
GaO             D0,Props: TPIS 1996 pt1 p214, pt2 p174
 2 tpis96 GA  1.00O   1.00    0.00    0.00    0.00 0   85.7224000     146823.607
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8925.107
 7.325543910D+04-9.804269510D+02 7.844122760D+00-7.171072850D-03 7.872780510D-06
-2.401464112D-09-2.594919458D-13               2.140581724D+04-1.799742951D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8925.107
 2.937313804D+06-1.118314112D+04 1.859366773D+01-6.854753450D-03 1.665399251D-06
-1.887560878D-10 7.972686920D-15               8.530248080D+04-9.904040480D+01
GaOH            Hf0,cons: TPIS 1996 pt1 p222; pt2 p178.
 2 tpis96 GA  1.00O   1.00H   1.00    0.00    0.00 0   86.7303400    -143630.495
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10583.608
 6.963101870D+04-1.247828695D+03 1.022001611D+01-5.922534390D-03 4.643387400D-06
-1.215936978D-09-2.945243614D-14               -1.275397794D+04-3.217063000D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10583.608
 8.429051010D+05-2.372324595D+03 8.009071090D+00 8.777230710D-05-5.943068910D-08
 9.841943440D-12-5.531552790D-16               -3.751788250D+03-2.171053719D+01
Ga2Br2          D0,cons: TPIS 1996 pt1 p244; pt2 p197.
 2 tpis96 GA  2.00BR  2.00    0.00    0.00    0.00 0  299.2540000    -136963.692
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20793.308
-1.117183241D+04-7.471471620D+01 1.030246084D+01-6.657929850D-04 8.200515850D-07
-5.297021520D-10 1.394553192D-13               -1.913297856D+04-1.317110316D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20793.308
-1.885373131D+04-1.263621802D+00 1.000108034D+01-4.774975660D-07 1.137227648D-10
-1.380820486D-14 6.690242430D-19               -1.951053843D+04-1.141667594D+01
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Ga2Br4          D0,Cons: TPIS 1996 pt1 p245; pt2 p198.
 2 tpis96 GA  2.00BR  4.00    0.00    0.00    0.00 0  459.0620000    -415820.034
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30591.766
-1.315545939D+04-4.136553020D+02 1.762849229D+01-3.514652160D-03 4.266937730D-06
-2.726515882D-09 7.118924490D-13              -5.283101810D+04-4.427520690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30591.766
-5.742167210D+04-7.160137370D+00 1.600598947D+01-2.608182270D-06 6.146455950D-10
-7.405438650D-14 3.567126630D-18              -5.493389760D+04-3.479271660D+01
Ga2Br6          Hf0,Cons: TPIS 1996 pt1 p246; pt2 p199.
 2 tpis96 GA  2.00BR  6.00    0.00    0.00    0.00 0  618.8700000    -673688.732
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       41151.266
-6.725116890D+03-8.067526550D+02 2.511671424D+01-6.636514570D-03 7.977555700D-06
-5.059685210D-09 1.313546388D-12              -8.370635200D+04-7.585278720D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       41151.266
-9.526173000D+04-1.444681880D+01 2.201192546D+01-5.145006740D-06 1.204348449D-09
-1.443806473D-13 6.928270740D-18              -8.782223300D+04-5.765895120D+01
Ga2CL2          Hf0,cons: Gurvich TPIS 1996 pt1 p237; pt2 p190.
 2 tpis96 GA  2.00CL  2.00    0.00    0.00    0.00 0  210.3514000    -220972.686
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19488.425
-9.246133700D+03-2.592159934D+02 1.102847129D+01-2.231983927D-03 2.720723456D-06
-1.743798624D-09 4.563666040D-13              -2.834059821D+04-2.067773700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19488.425
-3.668954200D+04-4.434580680D+00 1.000373051D+01-1.630793333D-06 3.853753320D-10
-4.652527730D-14 2.244498791D-18              -2.965633085D+04-1.469536245D+01
Ga2CL4          Hf0,cons: TPIS 1996 pt1 p237; pt2 p191.
 2 tpis96 GA  2.00CL  4.00    0.00    0.00    0.00 0  281.2568000    -602326.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       27315.392
 1.637343702D+04-1.140637354D+03 2.030139827D+01-8.997746200D-03 1.067254867D-05
-6.700290620D-09 1.725749144D-12              -7.162385010D+04-6.666362540D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       27315.392
-1.127110409D+05-2.138517542D+01 1.601738077D+01-7.415564640D-06 1.721694751D-09
-2.051361953D-13 9.797311500D-18              -7.746853380D+04-4.147281510D+01
Ga2CL6          Hf0,Cons: TPIS 1996 pt1 p238; pt2 p192.
 2 tpis96 GA  2.00CL  6.00    0.00    0.00    0.00 0  352.1622000    -962463.532
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       36359.799
 6.089469840D+04-2.104456302D+03 2.959653878D+01-1.537809796D-02 1.779096808D-05
-1.095619429D-08 2.779706493D-12              -1.118400535D+05-1.121945891D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       36359.799
-1.898445426D+05-4.413655240D+01 2.203505047D+01-1.470071128D-05 3.369512810D-09
-3.975462800D-13 1.884231868D-17              -1.226969998D+05-6.745333650D+01
Ga2F2           D0,cons: Gurvich TPIS 1996 pt1 p228; pt2 p183.
 2 tpis96 GA  2.00F   2.00    0.00    0.00    0.00 0  177.4428064    -606231.344
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17147.856
 2.978130650D+04-1.013975520D+03 1.374933053D+01-7.728050960D-03 9.064007330D-06
-5.641193220D-09 1.443106716D-12              -7.086083370D+04-4.109833950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17147.856
-8.773234930D+04-1.983775870D+01 1.001594030D+01-6.744402830D-06 1.556129063D-09
-1.845316975D-13 8.780884020D-18              -7.607368630D+04-1.908325521D+01
Ga2F4           D0,cons: TPIS 1996 pt1 p228; pt2 p184.
 2 tpis96 GA  2.00F   4.00    0.00    0.00    0.00 0  215.4396128   -1325002.958
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22653.242
 1.422079998D+05-2.798829941D+03 2.395904235D+01-1.293904774D-02 1.223101326D-05
-6.251209820D-09 1.334919195D-12              -1.496013710D+05-9.734153640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22653.242
-2.704366090D+05-1.049957196D+02 1.607903965D+01-3.178895920D-05 7.049582720D-09
-8.102379520D-13 3.760540530D-17              -1.644169589D+05-4.896591730D+01
Ga2F6           Hf0,Cons: TPIS 1996 pt1 p230; pt2 p185.
 2 tpis96 GA  2.00F   6.00    0.00    0.00    0.00 0  253.4364192   -2017623.843
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30131.476
 2.409045572D+05-4.142379800D+03 3.195773720D+01-1.297914290D-02 8.959282190D-06
-2.733621068D-09 1.554030994D-13              -2.272785240D+05-1.398403732D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30131.476
-4.368664800D+05-2.128208368D+02 2.215886373D+01-6.346287910D-05 1.399738556D-08
-1.601732039D-12 7.407584420D-17              -2.494298707D+05-7.787635830D+01
Ga2I2           D0,cons: Gurvich TPIS 1996 pt1 p252; pt2 p204.
 2 tpis96 GA  2.00I   2.00    0.00    0.00    0.00 0  393.2549400     13520.947
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21497.947
-8.960252670D+03-3.172057210D+01 1.012930491D+01-2.860191165D-04 3.535333010D-07
-2.289632389D-10 6.040085360D-14              -1.233174068D+03-9.801968380D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21497.947
-1.219056501D+04-5.287554470D-01 1.000045392D+01-2.011599344D-07 4.799467810D-11
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-5.834781080D-15 2.829565069D-19              -1.393258606D+03-9.052614910D+00
Ga2I4          D0,cons: TPIS 1996 pt1 p252; pt2 p205.
 2 tpis96 GA  2.00I   4.00    0.00    0.00    0.00 0  647.0638800    -159267.987
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       32583.813
-1.769495991D+04-1.354871509D+02 1.654625333D+01-1.199014713D-03 1.473754848D-06
-9.504796570D-10 2.499380837D-13              -2.333405795D+04-3.325712890D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       32583.813
-3.171299760D+04-2.287068836D+00 1.600194812D+01-8.588964380D-07 2.041966602D-10
-2.476145769D-14 1.198551944D-18              -2.401940505D+04-3.008672521D+01
Ga2I6          Hf0,Cons: TPIS 1996 pt1 p253; pt2 p206.
 2 tpis96 GA  2.00I   6.00    0.00    0.00    0.00 0  900.8728200    -317294.623
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       43573.378
-2.110891458D+04-3.695404160D+02 2.346811836D+01-3.189178210D-03 3.890339040D-06
-2.494830378D-09 6.532007280D-13              -4.301188090D+04-6.014811500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       43573.378
-6.015698150D+04-6.329209230D+00 2.200533040D+01-2.332008629D-06 5.513868480D-10
-6.659445350D-14 3.213670430D-18              -4.488699380D+04-5.161008750D+01
Ga2O           Hf0,cons: TPIS 1996 pt1 p216; pt2 p175.
 2 tpis96 GA  2.00O   1.00    0.00    0.00    0.00 0  155.4454000     -99457.457
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12162.595
 5.697197180D+04-8.074085990D+02 7.733061540D+00 1.478450874D-03-4.097743430D-06
 3.581158920D-09-1.107073202D-12              -9.512216820D+03-1.256149299D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12162.595
-1.193874986D+05-8.719341610D+01 7.064678200D+00-2.571524542D-05 5.651108490D-09
-6.448190540D-13 2.975374645D-17              -1.393694796D+04-6.942801300D+00
Ge             Hf:TPIS 1991 v2 pt1 p311. Spec:JPCRD v22 n5 1993 p1213.
 3 g 3/99 GE  1.00    0.00    0.00    0.00    0.00 0   72.6100000     367800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7398.584
-2.059215242D+04-1.432022103D+02 4.506002330D+00 1.547187840D-03-8.518296550D-06
 8.243824460D-09-2.566167305D-12              4.363070860D+04-6.225268510D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7398.584
-8.565413840D+05 3.917958660D+03-1.809888212D+00 2.276482224D-03-5.365627550D-07
 5.984958090D-11-2.541700646D-15              1.956518798D+04 3.841346790D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7398.584
 2.423965136D+07-2.543605174D+04 1.456087539D+01-2.592562254D-03 2.658628502D-07
-1.122785077D-11 1.620997559D-16              2.295812461D+05-8.953585860D+01
Ge+            JPCRD v22 n5 1993 p1213.
 3 g 3/99 GE  1.00E  -1.00    0.00    0.00    0.00 0   72.6094514    1134984.385
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.785
-3.453666430D+05 4.008449710D+03-1.522395737D+01 3.626030020D-02-3.351367260D-05
 1.431059219D-08-2.236976459D-12              1.157058042D+05 1.090151986D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.785
-2.244860570D+06 5.165531140D+03-3.867516510D-01 8.528730940D-04-1.386040003D-07
 1.155945775D-11-3.784413134D-16              1.006823985D+05 2.965783448D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.785
 5.768056240D+07-3.078606210D+04 8.706291820D+00-4.942233500D-04-2.690467703D-11
 1.853441677D-12-5.082067525D-17              3.857785420D+05-4.842599100D+01
Ge-            Spec:JPCRD v14 n3 1985 p731.
 3 g 3/99 GE  1.00E   1.00    0.00    0.00    0.00 0   72.6105486     245402.540
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6980.940
 2.989142308D+03 8.657417230D+01 2.191868507D+00 5.900795270D-04-6.375800580D-07
 3.661132150D-10-8.689778450D-14              2.835695190D+04 9.417004020D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6980.940
 1.352040246D+04-5.048518780D-01 2.500140247D+00-3.652944160D-09-6.716722200D-12
 1.378119925D-15-8.475212940D-20              2.881739757D+04 7.577334250D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6980.940
 1.079877187D+04 1.149969180D+00 2.499738027D+00 3.051383052D-08-1.930296476D-12
 6.305166240D-17-8.327676240D-22              2.880429709D+04 7.580847710D+00
GeBr           TPIS 1989 v2 pt1 p333; pt2 p287.
 2 g 7/95 GE  1.00BR  1.00    0.00    0.00    0.00 0  152.5140000     137440.771
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9866.131
-5.671557940D+04 9.168603580D+02-2.225065700D+00 2.172361330D-02-3.038886250D-05
 2.014978690D-08-5.214853240D-12              1.104508790D+04 4.108177040D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9866.131
-7.417995530D+05 2.259506430D+03 2.669469650D+00 9.305296040D-04-2.474333330D-07
 3.630579210D-11-1.815087790D-15              5.259595470D+02 1.939522540D+01
GeBr2          TPIS 1989 v2 pt1 p334; pt2 p288.
 2 tpis91 GE  1.00BR  2.00    0.00    0.00    0.00 0  232.4180000     -60962.897
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14193.463
-1.649738470D+03-2.296240010D+02 7.900161010D+00-1.936816750D-03 2.346091070D-06
-1.496594270D-09 3.902584250D-13              -8.316639570D+03-6.918410200D+00
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14193.463
-2.625559200D+04-4.322523600D+00 7.003708830D+00-1.659993690D-06 4.024870810D-10
-4.990764830D-14 2.472956460D-18              -9.482887810D+03-1.676535950D+00
GeBr3           TPIS 1989 v2 pt1 p335; pt2 p289.
 2 tpis91 GE  1.00BR  3.00    0.00    0.00    0.00 0  312.3220000    -119031.308
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18549.492
 2.725568677D+03-5.186213260D+02 1.199957754D+01-4.251024530D-03 5.103629720D-06
-3.233706250D-09 8.388358860D-13              -1.477988251D+04-2.534570086D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18549.492
-5.433926700D+04-9.280327950D+00 1.000765019D+01-3.297322150D-06 7.712929260D-10
-9.241571850D-14 4.432876230D-18              -1.742697092D+04-1.366960704D+01
GeBr4           TPIS 1989 v2 pt1 p336; pt2 p290.
 2 tpis91 GE  1.00BR  4.00    0.00    0.00    0.00 0  392.2260000    -291000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23963.218
 5.431940390D+03-6.777748800D+02 1.560015305D+01-5.507788880D-03 6.594764290D-06
-4.170146140D-09 1.080116643D-12              -3.557606400D+04-4.209134400D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23963.218
-6.977757910D+04-1.179873115D+01 1.300953955D+01-4.024938750D-06 9.203567210D-10
-1.076853369D-13 5.040954800D-18              -3.904148160D+04-2.689447543D+01
GeCL            TPIS, vol 2, part 1,1989 p314,328-30.
 2 g 7/95 GE  1.00CL  1.00    0.00    0.00    0.00 0  108.0627000      69027.753
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9596.668
 1.312624840D+04-5.792719460D+01 2.184913870D+00 1.313888930D-02-2.280992040D-05
 1.730687500D-08-4.942375070D-12               7.610395740D+03 1.395476780D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9596.668
-4.882693220D+05 1.657781490D+03 3.095819800D+00 7.281014850D-04-1.844853740D-07
 2.584610260D-11-1.212375290D-15              -3.657994580D+03 1.475058610D+01
GeCL2           TPIS 1989 v2 pt1 p334; pt2 p288.
 2 tpis91 GE  1.00CL  2.00    0.00    0.00    0.00 0  143.5154000    -171000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13276.791
 1.838480830D+04-5.827117660D+02 9.161352010D+00-4.464633870D-03 5.244653320D-06
-3.267916360D-09 8.367199170D-13              -1.975802720D+04-1.734324680D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13276.791
-4.886052250D+04-1.136952400D+01 7.009174690D+00-3.896423910D-06 9.019698450D-10
-1.072598220D-13 5.116839370D-18              -2.275184850D+04-4.657765720D+00
GeCL3           TPIS. DH: v2 pt1,1991 p331;Cons: v2 pts1&2,1979.
 2 g 8/95 GE  1.00CL  3.00    0.00    0.00    0.00 0  178.9681000    -266950.589
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17559.438
 1.935522440D+04-8.341563080D+02 1.312678860D+01-6.510788640D-03 7.695483410D-06
-4.818020280D-09 1.238264920D-12              -3.097240930D+04-3.552439620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17559.438
-7.594650070D+04-1.522999430D+01 1.001217930D+01-5.113704780D-06 1.168365870D-09
-1.370063360D-13 6.441790730D-18              -3.525492920D+04-1.719307590D+01
GeCL4           TPIS 1989 v2 pt1 p332; pt2 p286.
 2 tpis91 GE  1.00CL  4.00    0.00    0.00    0.00 0  214.4208000    -500000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21136.625
 6.502870410D+04-1.652482760D+03 1.881327000D+01-1.152426810D-02 1.310809980D-05
-7.961956110D-09 1.997505040D-12              -5.570052390D+04-6.754459960D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21136.625
-1.376261210D+05-3.603769500D+01 1.302816670D+01-1.164956960D-05 2.636193380D-09
-3.072926720D-13 1.439808750D-17              -6.426281780D+04-3.318180130D+01
GeF             TPIS, vol 2, part 1,1989 p314,324-25.
 2 g 7/95 GE  1.00F   1.00    0.00    0.00    0.00 0   91.6084032     -70591.091
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9144.823
 5.310368980D+04-4.832827930D+02 3.244976540D+00 1.180656030D-02-2.232084950D-05
 1.764180440D-08-5.174350360D-12              -6.885919070D+03 5.665087310D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9144.823
-4.324017740D+05 1.386361880D+03 3.359927390D+00 5.747584490D-04-1.381609050D-07
 1.825345200D-11-7.762330150D-16              -1.880857900D+04 1.121950790D+01
GeF2            TPIS 1989 v2 pt1 p326; pt2 p280.
 2 tpis91 GE  1.00F   2.00    0.00    0.00    0.00 0  110.6068064    -574000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11787.485
 7.543436100D+04-1.108505870D+03 9.079178910D+00-1.446428460D-03-6.563311550D-07
 1.474431870D-09-5.808473710D-13              -6.510661980D+04-2.200653180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11787.485
-1.275337580D+05-7.162740550D+01 7.053011560D+00-2.102898650D-05 4.612063520D-09
-5.253989710D-13 2.421225800D-17              -7.112637240D+04-8.484305710D+00
GeF3            TPIS. DH: v2 pt 1,1991 p323. Cons:v2 pts1&2,1979.
 2 g 8/95 GE  1.00F   3.00    0.00    0.00    0.00 0  129.6052096    -806332.833
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14678.187
 1.114063780D+05-1.776824770D+03 1.352119810D+01-2.982312270D-03-3.808958790D-08
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 1.623023050D-09-7.203558980D-13              -9.038302790D+04-4.568535760D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14678.187
-2.068970930D+05-1.112060300D+02 1.008254710D+01-3.282930850D-05 7.215790580D-09
-8.235194370D-13 3.800861430D-17              -9.999632740D+04-2.303648320D+01
GeF4            TPIS 1989 v2 pt1 p328; pt2 p282.
 2 tpis91 GE  1.00F   4.00    0.00    0.00    0.00 0  148.6036128   -1190150.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17293.024
 1.119833410D+05-1.636884040D+03 1.231387310D+01 1.025391530D-02-1.893686460D-05
 1.476764870D-08-4.324888390D-12              -1.374264000D+05-4.104320250D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17293.024
-3.253322220D+05-2.537713360D+02 1.318789010D+01-7.459931530D-05 1.637770110D-08
-1.867539100D-12 8.613732540D-17              -1.466180430D+05-4.122242070D+01
GeI             TPIS, vol 2, part 1,1989 p314,337-38.
 2 g 7/95 GE  1.00I   1.00    0.00    0.00    0.00 0  199.5144700     210975.084
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10010.445
-7.433304690D+04 1.033649640D+03-1.516944990D+00 1.553829630D-02-1.682005180D-05
 8.369568030D-09-1.548809480D-12               1.913013630D+04 3.959345320D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10010.445
-9.499873390D+05 2.470878430D+03 2.813092350D+00 8.430111900D-04-2.316964070D-07
 3.813339940D-11-2.056923220D-15               7.588118830D+03 1.947358070D+01
GeO             TPIS, vol 2, part 1,1989 p314-19.
 2 g 7/95 GE  1.00O   1.00    0.00    0.00    0.00 0   88.6094000     -37693.701
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8782.711
-5.705121810D+03 2.640641890D+02 6.993935570D-01 1.091588520D-02-1.474840000D-05
 9.889906430D-09-2.638982600D-12              -6.638849120D+03 2.111884970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8782.711
-2.160611930D+06 6.045062950D+03-2.472476150D+00 3.917074090D-03-1.083072890D-06
 1.347891010D-10-4.603478910D-15              -4.469941090D+04 5.049215340D+01
GeO2            TPIS 1989 v2 pt1 p323; pt2 p278.
 2 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 0  104.6088000    -106171.998
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11258.002
-3.824173830D+03 1.563451633D+02 1.694198285D+00 1.756205059D-02-2.418270032D-05
 1.632388154D-08-4.368957860D-12              -1.477534880D+04 1.556883504D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11258.002
-1.727347526D+05-2.961154443D+02 7.720726250D+00-8.824933390D-05 1.949874702D-08
-2.235834829D-12 1.036128507D-16              -1.387983288D+04-1.669888706D+01
GeS             TPIS, vol 2, part 1,1989 p314,344-45.
 2 g 7/95 GE  1.00S   1.00    0.00    0.00    0.00 0  104.6760000      92537.497
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9142.857
 3.499049510D+04-5.441195360D+02 6.040524820D+00-2.449802880D-03 2.313080070D-06
-1.159924440D-09 2.420251540D-13               1.263681730D+04-7.068825510D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9142.857
-3.566535440D+06 1.099738240D+04-8.971042610D+00 8.241849230D-03-2.600038250D-06
 3.962228400D-10-2.106449870D-14              -5.972355090D+04 9.768011130D+01
GeS2            TPIS 1989 v2 pt1 p347; pt2 p299.
 2 tpis91 GE  1.00S   2.00    0.00    0.00    0.00 0  136.7420000     118817.831
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13067.831
 5.543683600D+04-1.024826697D+03 1.057594552D+01-5.287883910D-03 5.295803080D-06
-2.872529530D-09 6.519027550D-13               1.735579668D+04-2.991750248D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13067.831
-8.970980360D+04-3.364377000D+01 7.525433720D+00-1.026368137D-05 2.282230718D-09
-2.628748770D-13 1.222218614D-17               1.195232103D+04-1.135201328D+01
Ge2             TPIS, vol 2, part 1,1989 p313-15.
 2 g 7/95 GE  2.00    0.00    0.00    0.00    0.00 0  145.2200000     471505.891
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10702.611
 2.137630630D+05-3.044332630D+03 1.868183170D+01-2.547250140D-02 2.196678340D-05
-8.415690800D-09 9.657757100D-13               7.015543000D+04-7.790904030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10702.611
 1.395098810D+06-3.279462000D+03 7.923080560D+00-1.528175390D-03 4.319451270D-07
-4.883547330D-11 1.977512520D-15               7.702689540D+04-1.895959060D+01
H               D0(H2):JMolSpc,v33 1970 p147. NSRDS-NBS 3 SEC 6 1972.
 3 g 6/97 H   1.00    0.00    0.00    0.00    0.00 0    1.0079400     217998.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               2.547370801D+04-4.466828530D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 6.078774250D+01-1.819354417D-01 2.500211817D+00-1.226512864D-07 3.732876330D-11
-5.687744560D-15 3.410210197D-19               2.547486398D+04-4.481917770D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.173757694D+08-1.312035403D+05 3.399174200D+01-3.813999680D-03 2.432854837D-07
-7.694275540D-12 9.644105630D-17               1.067638086D+06-2.742301051D+02
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H+              CP/R=2.5. IP: Moore,NSRDS-NBS 3,SEC 6,1972.
 3 g 8/96 H   1.00E  -1.00    0.00    0.00    0.00 0    1.0073914    1536245.928
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.840214877D+05-1.140646644D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.840214877D+05-1.140646644D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.840214877D+05-1.140646644D+00
H-              JPCRD v14 n3 1985 p731.
 3 g 9/96 H   1.00E   1.00    0.00    0.00    0.00 0    1.0084886     139031.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.597615494D+04-1.139013868D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.597615494D+04-1.139013868D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.597615494D+04-1.139013868D+00
HALO            Hform & cons: Gurvich TPIS 1996 pt1 p147; pt2 p111.
 2 tpis96 AL  1.00O   1.00H   1.00    0.00    0.00 0   43.9888780       1821.114
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9935.217
 2.668608286D+04-4.663132990D+02 5.383760360D+00 2.902519494D-03-2.244844823D-07
-1.516222095D-09 6.951560420D-13                1.235874429D+03-6.508610344D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9935.217
 7.845718980D+04-1.515584535D+03 8.572733110D+00-4.142402230D-04 8.934546000D-08
-1.006967493D-11 4.607666790D-16                6.662952540D+03-2.672917163D+01
HALO2           Hform & cons: Gurvich TPIS 1996 pt1 p148; pt2 p112.
 2 tpis96 H   1.00AL  1.00O   2.00    0.00    0.00 0   59.9882780    -355473.551
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11980.604
 3.544598910D+03 1.159819104D+02 8.637970690D-01 2.460875785D-02-3.423160120D-05
 2.373182987D-08-6.467608830D-12                -4.449506140D+04 2.012317063D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11980.604
 6.985705440D+05-2.864935042D+03 1.086721494D+01-5.368312700D-05-2.836877559D-08
 6.291641190D-12-3.889033110D-16                -2.764392495D+04-3.775886342D+01
HBO             Boron oxide-hydride .Cons&Hf0:TPIS1996 pt1 p39, pt2 p23.
 2 tpis96 H   1.00B   1.00O   1.00    0.00    0.00 0   27.8183400    -210621.205
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9166.898
 6.360975030D+04-8.001557590D+02 6.218816130D+00-7.801679980D-04 3.141286759D-06
-2.031853478D-09 3.738552890D-13                -2.240282910D+04-1.326952393D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9166.898
 8.861860230D+05-3.913068050D+03 9.888644800D+00-8.222269140D-04 1.621530554D-07
-1.703550237D-11 7.372740020D-16                -3.161852029D+03-4.036812720D+01
HBO+
 2 J12/75 H   1.00B   1.00O   1.00E  -1.00    0.00 0   27.8177914    1187574.534
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.254428300D+00 8.030187200D-03-5.974907200D-06
 2.428195000D-09-4.305112400D-13                1.418506900D+05 1.081220760D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.947508000D+00 3.431543600D-03-1.278708400D-06
 2.218060400D-10-1.475719200D-14                1.413599800D+05 1.998895970D+00
HBO-
 2 J12/75 H   1.00B   1.00O   1.00E   1.00    0.00 0   27.8188886    -244477.956
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.970795500D+00-2.210010700D-03 1.453541300D-05
-1.563892500D-08 5.397896600D-12                -3.058949900D+04 4.824969670D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.086926500D+00 2.978475600D-03-1.238710700D-06
 2.469333500D-10-1.845504800D-14                -3.093002600D+04 2.780142470D+00
HBO2            Cons & Hf0: TPIS 1996 pt1 p42 pt2 p26.
 2 tpis96 H   1.00B   1.00O   2.00    0.00    0.00 0   43.8177400    -560210.053
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10918.102
 6.225087470D+03 7.566153690D+01 1.253406833D+00 1.748006535D-02-1.982688351D-05
 1.229656460D-08-3.153609847D-12                -6.878588780D+04 1.767793507D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10918.102
 1.049369185D+06-4.479145480D+03 1.197755861D+01-4.735743400D-04 6.080207140D-08
-3.641565440D-12 6.155973170D-17                -4.221149470D+04-4.911366820D+01
HBS
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 2 J12/75 H   1.00B   1.00S   1.00    0.00    0.00 0   43.8849400      50208.558
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.559590300D+00 1.396683800D-02-1.798859500D-05
 1.231514100D-08-3.409095700D-12                 5.089093600D+03 1.350189860D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.441226500D+00 2.997982500D-03-1.193823000D-06
 2.119583200D-10-1.346609700D-14                 4.440297500D+03-6.467831740D-01
HBS+
 2 J12/75 H   1.00B   1.00S   1.00E  -1.00    0.00 0   43.8843914    1129498.895
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.251156100D+00 1.207716800D-02-1.532215600D-05
 1.049409000D-08-2.932529200D-12                 1.347547600D+05 1.127076990D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.709754200D+00 2.818703600D-03-1.163308800D-06
 2.176883900D-10-1.510868600D-14                 1.341913900D+05-8.374721460D-01
HBr             TPIS 1989 v1 pt1 p205;  pt2 p106.
 2 tpis89 H   1.00BR  1.00    0.00    0.00    0.00 0   80.9119400     -36290.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8648.104
 2.527222498D+04-4.065110270D+02 6.043116610D+00-7.717882870D-03 1.149123213D-05
-7.293633280D-09 1.747406491D-12 0.000000000D+00-3.510414550D+03-9.903186290D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8648.104
 1.170033949D+06-3.786521010D+03 7.503148050D+00-1.284963943D-03 3.206257190D-07
-3.444925160D-11 1.126758417D-15 0.000000000D+00 1.856413349D+04-2.562712911D+01
HCN             Cons and Hf0: TPIS,v2 pt1,1978 p32.
 2 g 7/88 H   1.00C   1.00N   1.00    0.00    0.00 0   27.0253800     135000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9235.463
 9.098297830D+04-1.238659660D+03 8.721322290D+00-6.528281280D-03 8.872747230D-06
-4.808908770D-09 9.317917730D-13                 2.121978990D+04-2.746686680D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9235.463
 1.236898250D+06-4.446761840D+03 9.738911630D+00-5.855398100D-04 1.072855010D-07
-1.013403600D-11 3.348736660D-16                 4.244594810D+04-4.005800750D+01
HCO             HF: Chem.Phys.Let.v258,1996 p626. Cons:JPCRD v17,1988 p296.
 2 g 9/96 H   1.00C   1.00O   1.00    0.00    0.00 0   29.0180400      42397.850
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9989.450
-1.189906845D+04 2.151611774D+02 2.730183950D+00 1.806621526D-03 4.984153050D-06
-5.814462670D-09 1.869659718D-12                 2.905719059D+03 1.136793477D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9989.450
 6.911335700D+05-3.643217800D+03 9.587084880D+00-1.104891812D-03 2.829488544D-07
-3.537972860D-11 1.739690104D-15                 2.535622651D+04-3.570198702D+01
HCO+            FORMYL ION.  JANAF, 12/70 INPUT.
 3 J12/70 H   1.00C   1.00O   1.00E  -1.00    0.00 0   29.0174914     833000.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9254.415
 1.183165170D+05-1.604667620D+03 1.067171220D+01-1.168899320D-02 1.614949320D-05
-9.978314210D-09 2.376297120D-12                 1.069395710D+05-3.820339851D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9254.415
 1.203649250D+06-4.460980190D+03 9.932598010D+00-7.540749800D-04 1.351582400D-07
-1.302833390D-11 5.221060670D-16                 1.263492120D+05-4.106699341D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9254.415
-1.518062380D+06-5.526680780D+02 7.610715960D+00-1.185435840D-05 7.050967100D-10
-2.195936690D-14 2.791470700D-19                 9.874460220D+04-2.305471671D+01
HCCN            Cons and Hf0: TPIS v2 pt1,1989 p228.
 2 tpis89 H   1.00C   2.00N   1.00    0.00    0.00 0   39.0360800     610430.628
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11865.730
 2.992851400D+03-4.404483970D+02 6.939939300D+00 3.846576010D-03-1.265137940D-06
-3.636043180D-10 2.747926430D-13                 7.370870140D+04-1.315250732D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11865.730
 9.395761840D+05-4.091115680D+03 1.272239200D+01-6.874741130D-04 1.231265150D-07
-1.187086160D-11 4.761286670D-16                 9.585194840D+04-5.248739832D+01
HCL             TPIS 1989 v1 pt1 p186; pt2 p93.
 2 tpis89 H   1.00CL  1.00    0.00    0.00    0.00 0   36.4606400     -92310.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8640.104
 2.062588287D+04-3.093368855D+02 5.275418850D+00-4.828874220D-03 6.195794600D-06
-3.040023782D-09 4.916790030D-13 0.000000000D+00-1.067782299D+04-7.309317750D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8640.104
 9.157749510D+05-2.770550211D+03 5.973539790D+00-3.629810060D-04 4.735529190D-08
 2.810262054D-12-6.656104220D-16 0.000000000D+00 5.674958050D+03-1.642827056D+01
HD              TPIS 1989 v1 pt1 p144; pt2 p53.
 3 tpis89 H   1.00D   1.00    0.00    0.00    0.00 0    3.0220420       323.302
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8509.102
 2.519120338D+04-2.761004999D+02 4.644441290D+00-2.082376844D-03 1.418070803D-06
 2.839893835D-10-3.202331030D-13                 3.913616430D+02-9.395396120D+00
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8509.102
 8.455830000D+05-1.956578537D+03 4.404373870D+00 5.751681090D-04-2.131983152D-07
 4.036126680D-11-2.727170705D-15                 1.227254163D+04-1.084742878D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8509.102
 4.829960940D+08-3.077144916D+05 7.864816510D+01-8.332990910D-03 4.732254110D-07
-1.372721571D-11 1.614120677D-16                 2.431070386D+06-6.569437060D+02
HD+
 2 J 9/77 H   1.00D   1.00E  -1.00    0.00    0.00 0    3.0214934    1496830.497
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.882713600D+00-3.077938100D-03 8.191447300D-06
-6.811949900D-09 1.985989800D-12                 1.789456300D+05-2.803359780D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.290976400D+00 1.155152900D-03-3.444946300D-07
 7.672268200D-11-8.094813300D-15                 1.789427900D+05-4.786072120D-01
HD-
 2 J 9/77 H   1.00D   1.00E   1.00    0.00    0.00 0    3.0225906     235489.461
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.642887700D+00-2.129128900D-03 8.928412300D-06
-9.348120400D-09 3.256497100D-12                 2.726927100D+04-2.255626610D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.493994900D+00 1.244866700D-03-4.728871400D-07
 9.105963700D-11-6.486292600D-15                 2.715773400D+04-2.231104610D+00
HDO             TPIS 1989 v1 pt1 p145; pt2 p55.
 2 g 5/99 H   1.00D   1.00O   1.00    0.00    0.00 0   19.0214420    -245280.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9925.723
-2.737795356D+04 4.310503900D+02 1.558479899D+00 5.764969150D-03-4.855129360D-06
 3.382990170D-09-1.040863879D-12                -3.273226450D+04 1.487751891D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9925.723
 1.711376798D+06-5.322872300D+03 9.124351520D+00-3.400664150D-04 4.152343520D-08
-4.780768570D-14-1.468035170D-16                 3.245224680D+03-3.774600680D+01
HDO2            TPIS, vol 1, part 1,1989 p142,146-47, NRRAO1.
 2 g 5/95 H   1.00D   1.00O   2.00    0.00    0.00 0   35.0208420    -140231.741
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11334.965
-3.216499650D+04 7.492367220D+02-1.957694050D+00 2.412807570D-02-2.915953440D-05
 1.930021120D-08-5.226999680D-12                -2.150941750D+04 3.672416710D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11334.965
 1.313170990D+06-5.175614850D+03 1.216489120D+01-6.136626350D-04 1.227543920D-07
-1.079602190D-11 3.873860270D-16                 1.303313850D+04-5.085262990D+01
HDO2            TPIS 1989 v1 pt1 p146; pt2 p56.
 2 g 5/99 H   1.00D   1.00O   2.00    0.00    0.00 0   35.0208420    -140241.635
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11334.965
-3.216476650D+04 7.492334460D+02-1.957676212D+00 2.412802791D-02-2.915946684D-05
 1.930016324D-08-5.226986310D-12                -2.151059175D+04 3.672406740D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11334.965
 1.313180619D+06-5.175637120D+03 1.216490975D+01-6.136699480D-04 1.227560176D-07
-1.079624939D-11 3.874013720D-16                 1.303209670D+04-5.085276870D+01
HF              TPIS 1989 v1 pt1 p162; pt2 p77.
 3 tpis89 H   1.00F   1.00    0.00    0.00    0.00 0   20.0063432    -273300.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8599.103
-3.192098970D+03 5.986807720D+01 3.055113902D+00 1.684673783D-03-3.287394830D-06
 3.095923617D-09-9.764691610D-13 0.000000000D+00-3.418443160D+04 3.294904120D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8599.103
 7.257089040D+05-1.484797741D+03 3.855527470D+00 7.138989850D-04-2.106757333D-07
 3.050092453D-11-1.639495583D-15 0.000000000D+00-2.355456660D+04-3.203856830D+00
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8599.103
 1.764588423D+08-8.789998060D+04 1.886524859D+01-6.850866180D-04-1.403468022D-08
 1.503711045D-12-2.717518148D-17 0.000000000D+00 6.853573220D+05-1.393231574D+02
HI
 2 J 9/61 H   1.00I   1.00    0.00    0.00    0.00 0  127.9124100      26359.556
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.696372200D+00-1.422475500D-03 3.013118800D-06
-1.266640300D-09-3.509876500D-14                 2.107358100D+03 4.088121110D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.910400800D+00 1.568818800D-03-5.922763200D-07
 1.053709400D-10-7.037511600D-15                 2.250865900D+03 7.864470510D+00
HNC             Cons: Jacox,1988.  Hf: TPIS,vol,2 pt 1,1991.
 2 g11/92 H   1.00N   1.00C   1.00    0.00    0.00 0   27.0253800     194378.121
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10000.724
 4.870404530D+04-9.891138220D+02 9.721970560D+00-1.113540800D-02 1.668780870D-05
-1.113877210D-08 2.893404130D-12                 2.664664620D+04-3.104726610D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10000.724
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 1.198765940D+06-3.918875320D+03 9.117953120D+00-3.417426590D-04 3.313953030D-08
-5.690989560D-13-7.794339270D-17              4.658767040D+04-3.468528650D+01
HNCO            Hydrogen isocyanate. JANAF 1970.JCP v99 1993 p4638.
 2 g 2/96 H   1.00N   1.00C   1.00O   1.00    0.00 0   43.0247800    -118061.400
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10961.254
 7.571219620D+04-9.556385640D+02 6.708321880D+00 4.774600340D-03-5.088271630D-06
 3.807390230D-09-1.201806525D-12              -1.067496288D+04-1.357685941D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10961.254
 1.257367696D+06-5.038239730D+03 1.249617398D+01-6.975327400D-04 1.117432856D-07
-9.539825840D-12 3.352825210D-16              1.463698265D+04-5.320579852D+01
HNO             TPIS 1989 v1 pt1 p362;pt2 p227. JPCRD 1988 v17 p301.
 2 g 5/99 H   1.00N   1.00O   1.00    0.00    0.00 0   31.0140800     102032.725
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9941.880
-6.854790880D+04 9.551653430D+02-6.000761550D-01 7.995138190D-03-6.545236720D-07
-3.670814670D-09 1.783565723D-12              6.435337270D+03 3.048170024D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9941.880
-5.797632990D+06 1.946313410D+04-2.153876091D+01 1.798321221D-02-4.978774100D-06
 6.401747790D-10-3.144626897D-14              -1.104709471D+05 1.819552443D+02
HNO2            Cis-trans.Hf0,Cons:TPIS 1989 v1 pt1 p363;pt2 p228.
 2 tpis89 H   1.00N   1.00O   2.00    0.00    0.00 0   47.0134800     -78451.922
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11597.285
 8.591985060D+03 1.203644046D+02 9.412979120D-01 1.942891839D-02-2.253174194D-05
 1.384587594D-08-3.473550460D-12              -1.106337202D+04 2.073967459D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11597.285
 8.787904130D+05-3.990455030D+03 1.187349269D+01-4.881900610D-04 7.133636790D-08
-5.376303340D-12 1.581778986D-16              1.246343241D+04-4.608874560D+01
HNO3            Hf0,Cons: TPIS 1989 v1 pt1 p367; pt2 p231.
 2 g 5/99 H   1.00N   1.00O   3.00    0.00    0.00 0   63.0128800    -133912.869
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11876.390
 9.202869010D+03 1.093774496D+02-4.521042450D-01 2.984914503D-02-3.190635500D-05
 1.720931528D-08-3.782649830D-12              -1.764048507D+04 2.746644974D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11876.390
-9.497809640D+04-2.733024468D+03 1.449426995D+01-7.821868050D-04 1.702693665D-07
-1.930543961D-11 8.870455120D-16              -4.882517780D+03-5.928392890D+01
HOCL            TPIS, vol 1 part 1,1989 p.184 and 187-88.
 2 tpis89 H   1.00O   1.00CL  1.00    0.00    0.00 0   52.4600400     -75740.849
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10223.809
-9.892422080D+03 3.569044430D+02 1.442940270D-01 1.618245610D-02-2.179994870D-05
 1.508707150D-08-4.123194400D-12              -1.177370310D+04 2.479303640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10223.809
 8.532389090D+05-2.849447670D+03 7.949826710D+00-1.055179780D-04-1.467915450D-08
 4.574952700D-12-3.052330800D-16              7.260868110D+03-2.250834380D+01
HOF             TPIS, VOL 1, PART 1, PAGES 164 AND 171-72.
 2 tpis89 H   1.00O   1.00F   1.00    0.00    0.00 0   36.0057432     -96898.221
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10088.435
-3.696937930D+04 7.809077120D+02-2.077724310D+00 2.038701040D-02-2.586936270D-05
 1.713810000D-08-4.551320180D-12              -1.631723450D+04 3.645074180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10088.435
 8.811850280D+05-3.119970510D+03 8.223668430D+00-2.297834420D-04 1.458600850D-08
 1.096541040D-12-1.404775820D-16              6.300268330D+03-2.590120020D+01
HO2             Hills JCP 1984 v81 p4458. Jacox JPCRD 1988 v17 p303.
 2 g 5/99 H   1.00O   2.00    0.00    0.00    0.00 0   33.0067400      12552.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10002.162
-7.598882540D+04 1.329383918D+03-4.677388240D+00 2.508308202D-02-3.006551588D-05
 1.895600056D-08-4.828567390D-12              -5.809366430D+03 5.193602140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10002.162
-1.810669724D+06 4.963192030D+03-1.039498992D+00 4.560148530D-03-1.061859447D-06
 1.144567878D-10-4.763064160D-15              -3.194418740D+04 4.066850920D+01
HO2-            TPIS 1989 v1 pt1 p121; pt2 p35.
 2 tpis89 H   1.00O   2.00E   1.00    0.00    0.00 0   33.0072886     -97629.980
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10017.620
 5.980517650D+02 4.532183650D+02-7.885641820D-01 1.660606821D-02-2.000303995D-05
 1.273201256D-08-3.271493480D-12              -1.467223832D+04 2.880195356D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10017.620
 8.883563120D+05-3.269606190D+03 8.381873830D+00-3.027048578D-04 3.189230840D-08
-9.694896340D-13-4.235596680D-17              7.066473970D+03-2.750636195D+01
HPO             Hf0:TPIS 1989 v1 pt1 p424.Spec:JPCRD 1988 v17 n2 p269.
 2 tpis89 H   1.00P   1.00O   1.00    0.00    0.00 0   47.9811010     -56868.759
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10065.343
-3.816314120D+04 7.927641870D+02-1.889940652D+00 1.800907425D-02-1.857631793D-05
 1.018768867D-08-2.355583619D-12 0.000000000D+00-1.157641240D+04 3.692925910D+01
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   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10065.343
 3.842459450D+05-2.434951707D+03 8.582173920D+00-4.058448570D-04-1.669488740D-08
 2.253640566D-11-1.943063011D-15 0.000000000D+00 5.761632120D+03-2.649097544D+01
HSO3F
 2 J 6/72 H   1.00S   1.00O   3.00F   1.00    0.00 0  100.0705432    -753129.062
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.119244500D+00 3.154571000D-02-3.131788800D-05
 1.246150700D-08-8.251463000D-13                -9.236159600D+04 1.555969560D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.036419000D+01 5.386116400D-03-2.123157200D-06
 3.820834300D-10-2.580709000D-14                -9.439833400D+04-2.600550340D+01
H2              Hydrogen. TPIS, v1, pt2, 1978, pp31-32.
 3 tpis78 H   2.00    0.00    0.00    0.00    0.00 0    2.0158800         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8468.102
 4.078322810D+04-8.009185450D+02 8.214701670D+00-1.269714360D-02 1.753604930D-05
-1.202860160D-08 3.368093160D-12                2.682484380D+03-3.043788660D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8468.102
 5.608123380D+05-8.371491340D+02 2.975363040D+00 1.252249930D-03-3.740718420D-07
 5.936628250D-11-3.606995730D-15                5.339815850D+03-2.202764050D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8468.102
 4.966716130D+08-3.147448120D+05 7.983887500D+01-8.414504190D-03 4.753060440D-07
-1.371809730D-11 1.605374600D-16                2.488354660D+06-6.695524190D+02
H2+             TPIS, vol 1, part 2,1978 p33.
 3 tpis78 H   2.00E  -1.00    0.00    0.00    0.00 0    2.0153314    1494672.430
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8583.103
-3.120892210D+04 2.304629950D+02 3.335561190D+00-2.419049150D-03 7.006012610D-06
-5.610004250D-09 1.564168040D-12                1.774104600D+05-8.278338450D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8583.103
 1.672226180D+06-6.595185440D+03 1.279321970D+01-5.509345460D-03 2.030669460D-06
-3.351027540D-10 1.946089130D-14                2.189999580D+05-6.792711090D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8583.103
-1.822062020D+08 1.018191290D+05-1.245820750D+01 1.076634640D-03-3.932209660D-08
 6.285143440D-13-2.094378960D-18                -6.513061550D+05 1.471405610D+02
H2-
 2 J 9/77 H   2.00E   1.00    0.00    0.00    0.00 0    2.0164286     235376.895
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.838014200D+00-3.179476800D-03 1.004301100D-05
-9.551811600D-09 3.128133000D-12                2.723485600D+04-3.998623600D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.292107600D+00 1.435862600D-03-5.470559300D-07
 1.043388300D-10-7.382799800D-15                2.721618100D+04-1.982777700D+00
HBOH            Cons & D0: TPIS 1996 pt1 p44 pt2 p27.
 2 g 9/98 H   2.00B   1.00O   1.00    0.00    0.00 0   28.8262800     -48724.364
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10940.536
-6.159644190D+04 1.223483035D+03-5.460370510D+00 3.555388680D-02-4.675020140D-05
 3.236008850D-08-8.986053320D-12                -1.263659051D+04 5.422352290D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10940.536
 1.534611049D+06-5.753666430D+03 1.270893665D+01-7.059628250D-04 1.027679375D-07
-7.670926740D-12 2.211854768D-16                2.779370419D+04-5.608860080D+01
HCHO,formaldehy   Cons: TPIS, 1979. Hf:TRC,w5300,6/78.
 2 g 8/88 H   2.00C   1.00O   1.00    0.00    0.00 0   30.0259800    -108580.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10019.717
-1.173922110D+05 1.873636547D+03-6.890327710D+00 2.641571472D-02-2.186402425D-05
 1.005702110D-08-2.023502935D-12                -2.307355518D+04 6.420441192D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10019.717
 1.700799002D+06-7.620786660D+03 1.472440991D+01-1.649079928D-03 3.292063320D-07
-3.494945200D-11 1.526081986D-15                3.146769107D+04-7.386432128D+01
HCOOH           Formic acid. JPCRD vol 7, no 1, 1978, P363.
 2 g 8/88 H   2.00C   1.00O   2.00    0.00    0.00 0   46.0253800    -378570.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10927.649
-2.906331910D+04 7.658449340D+02-3.328450010D+00 2.817551970D-02-2.370062730D-05
 1.166071690D-08-2.791394720D-12                -5.006446900D+04 4.387113544D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10927.649
 4.872179250D+05-7.632196980D+03 2.132783990D+01-4.402525040D-03 1.101995700D-06
-1.364334930D-10 6.648380880D-15                -5.781698870D+03-1.111787766D+02
H2F2            TPIS 1989  v1 pt1 p164; pt2 p308.
 2 tpis89 H   2.00F   2.00    0.00    0.00    0.00 0   40.0126864    -569923.778
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13869.430
 5.259214710D+04-9.913544890D+02 1.043577115D+01-2.407796033D-03-6.376956160D-07
 2.735784900D-09-1.104348590D-12 0.000000000D+00-6.572460830D+04-3.038432132D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13869.430
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 1.464995601D+06-3.335074920D+03 9.187487040D+00 1.051127249D-03-3.278605570D-07
 4.456046230D-11-2.281370136D-15 0.000000000D+00-4.825442090D+04-2.639128168D+01
H2O             CODATA 1989. JRNBS 1987 v92 p35. TRC tuv-25 10/88.
 2 g 8/89 H   2.00O   1.00    0.00    0.00    0.00 0   18.0152800    -241826.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9904.092
-3.947960830D+04 5.755731020D+02 9.317826530D-01 7.222712860D-03-7.342557370D-06
 4.955043490D-09-1.336933246D-12 0.000000000D+00-3.303974310D+04 1.724205775D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9904.092
 1.034972096D+06-2.412698562D+03 4.646110780D+00 2.291998307D-03-6.836830480D-07
 9.426468930D-11-4.822380530D-15 0.000000000D+00-1.384286509D+04-7.978148510D+00
H2O+            TPIS 1989 v1 pt1 p125; pt2 p38.
 3 tpis89 H   2.00O   1.00E  -1.00    0.00    0.00 0   18.0147314     981600.966
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9934.466
-4.214391040D+04 6.753570570D+02-1.967713310D-02 1.071692304D-02-1.280882024D-05
 9.210121900D-09-2.653367317D-12 0.000000000D+00 1.136952737D+05 2.293664418D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9934.466
 6.265955080D+05-2.873551651D+03 7.726361570D+00-9.069268960D-04 6.187757820D-07
-1.202750679D-10 7.414123600D-15 0.000000000D+00 1.342694699D+05-2.643064569D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9934.466
-1.753918756D+07-2.632704308D+03 1.165527354D+01-7.730080770D-04 5.630312640D-08
-1.964863168D-12 2.681675399D-17 0.000000000D+00 1.168168383D+05-5.762628710D+01
H2O2            Cons:TPIS 1978 v1 pt1 p121.Hf:TPIS 1989 v1 pt1 p127.
 2 g 6/99 H   2.00O   2.00    0.00    0.00    0.00 0   34.0146800    -135880.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11158.835
-9.279533580D+04 1.564748385D+03-5.976460140D+00 3.270744520D-02-3.932193260D-05
 2.509255235D-08-6.465045290D-12 0.000000000D+00-2.494004728D+04 5.877174180D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11158.835
 1.489428027D+06-5.170821780D+03 1.128204970D+01-8.042397790D-05-1.818383769D-08
 6.947265590D-12-4.827831900D-16 0.000000000D+00 1.418251038D+04-4.650855660D+01
H2S             TPIS 1989 v1 pt1 p298; pt2 p181.
 2 tpis89 H   2.00S   1.00    0.00    0.00    0.00 0   34.0818800     -20600.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9957.120
 1.197021744D+04-1.028938513D+02 4.239946370D+00-8.018112670D-04 4.476419880D-06
-2.747742643D-09 4.527488180D-13 0.000000000D+00-3.114034739D+03 3.807634460D-01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9957.120
 1.432316933D+06-5.290965660D+03 1.016831761D+01-9.721306840D-04 2.119657690D-07
-2.180371327D-11 9.372858230D-16 0.000000000D+00 2.913139316D+04-4.354201970D+01
H2SO4           TPIS 1989 v1 pt1 p300; pt 2 p182.
 2 tpis89 H   2.00S   1.00O   4.00    0.00    0.00 0   98.0794800    -732731.721
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16508.589
-4.129150050D+04 6.681589890D+02-2.632753507D+00 5.415382480D-02-7.067502230D-05
 4.684611420D-08-1.236791238D-11 0.000000000D+00-9.315660120D+04 3.961097730D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16508.589
 1.437877914D+06-6.614902530D+03 2.157662058D+01-4.806255970D-04 3.010775121D-08
 2.334842469D-12-2.946330375D-16 0.000000000D+00-5.259092950D+04-1.023603571D+02
H2BOH           Cons & Hf0: TPIS 1996 pt1 p46 pt2 p29.
 2 tpis96 H   3.00B   1.00O   1.00    0.00    0.00 0   29.8342200    -289633.898
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10622.306
-8.686766780D+04 1.820335089D+03-1.032373881D+01 4.922801060D-02-5.978619910D-05
 3.946062730D-08-1.068442257D-11               -4.415238150D+04 7.986177290D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10622.306
 2.294795193D+06-9.382923560D+03 1.798228329D+01-1.506116214D-03 2.635641095D-07
-2.483163637D-11 9.736759120D-16               2.039738953D+04-9.448201210D+01
HB(OH)2         Cons & Hf0: TPIS 1996 pt1 p47 pt2 p30.
 2 tpis96 H   3.00B   1.00O   2.00    0.00    0.00 0   45.8336200    -644438.724
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12157.532
-2.067044022D+04 9.534459160D+02-8.088956520D+00 5.972425290D-02-8.071336320D-05
 5.612118350D-08-1.553607566D-11               -8.264270810D+04 6.539571640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12157.532
 2.122674609D+06-8.615948940D+03 1.966179520D+01-8.148411500D-04 8.955082040D-08
-3.344830510D-12-6.919578140D-17               -2.788790377D+04-9.983559610D+01
H3BO3           Cons & Hsubl(0): TPIS 1996 pt1 p50 pt2 p32.
 2 tpis96 H   3.00B   1.00O   3.00    0.00    0.00 0   61.8330200    -1004360.442
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13559.958
 2.568901843D+04 1.138029495D+02-4.045096580D+00 5.924521680D-02-8.148028410D-05
 5.658593290D-08-1.549277050D-11               -1.221702050D+05 4.132220140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13559.958
 2.297369132D+06-8.933571790D+03 2.193496552D+01-3.094783490D-04-5.064052990D-08
 1.482296684D-11-9.764420900D-16               -6.970298470D+04-1.122292829D+02
H3B3O3          Cons & Hf0: TPIS 1996 pt1 p53 pt2 p34.
 2 tpis96 H   3.00B   3.00O   3.00    0.00    0.00 0   83.4550200    -1203760.987
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15603.321
-1.985284188D+05 4.104132090D+03-2.827215617D+01 1.269639253D-01-1.558505781D-04
 9.966304070D-08-2.603677650D-11                -1.648494375D+05 1.763917407D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15603.321
 1.286220713D+06-1.093258784D+04 3.213518670D+01-2.595402269D-03 5.353766470D-07
-5.833567380D-11 2.600757913D-15                -8.752856890D+04-1.770847815D+02
H3B3O6          Cons & Hf0: TPIS 1996 pt1 p55 pt2 p35.
 2 tpis96 H   3.00B   3.00O   6.00    0.00    0.00 0  131.4532200   -2263687.611
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23696.853
-2.067031503D+04 7.083391540D+02-7.123820950D+00 1.025049979D-01-1.295004602D-04
 8.322737590D-08-2.145746724D-11                -2.778049216D+05 6.063597630D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23696.853
 1.952433352D+06-1.154932896D+04 3.892676110D+01-1.113852280D-03 1.280317726D-07
-5.728464820D-12-2.214529572D-17                -2.120927136D+05-2.075566801D+02
H3F3            TPIS 1989 v1 pt1 p166; pt 2 p309.
 2 tpis89 H   3.00F   3.00    0.00    0.00    0.00 0   60.0190296    -883676.790
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15263.022
 9.888562650D+04-1.380212880D+03 8.980458470D+00 1.871609057D-02-3.127862508D-05
 2.589436165D-08-8.040372270D-12 0.000000000D+00-1.013661491D+05-2.585302557D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15263.022
 2.515790373D+06-8.789423320D+03 2.023933445D+01-1.131704646D-03 1.692779921D-07
-1.308662105D-11 3.978322000D-16 0.000000000D+00-5.471713650D+04-9.907787640D+01
H3O+            TPIS 1989 v1 pt1 p130; pt2 p41.
 3 tpis89 H   3.00O   1.00E  -1.00    0.00    0.00 0   19.0226714     598000.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10046.427
-7.927361690D+04 1.321886357D+03-4.305089630D+00 2.306754819D-02-2.516149900D-05
 1.596119352D-08-4.162293010D-12 0.000000000D+00 6.457600350D+04 4.585347990D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10046.427
 2.961335277D+06-9.200996930D+03 1.342845304D+01-5.658383500D-04 1.307422780D-08
 7.048453350D-12-6.028985800D-16 0.000000000D+00 1.291539395D+05-7.032434620D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10046.427
-1.586888366D+07 4.874114080D+03 8.887519270D+00 1.290694156D-04-8.104008490D-09
 2.623758985D-13-3.433908740D-18 0.000000000D+00 2.109743132D+04-3.222997220D+01
(HCOOH)2        Formic acid dimer. Cons & Hf298: JPCRD v7,n1,1978 p363.
 2 g 8/88 H   4.00C   2.00O   4.00    0.00    0.00 0   92.0507600    -820942.640
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19631.909
-2.001477350D+05 3.502503660D+03-1.853516560D+01 9.547554670D-02-1.059198650D-04
 6.323201900D-08-1.567597850D-11                -1.172623860D+05 1.319662344D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19631.909
 3.308073030D+06-1.633631890D+04 3.751305360D+01-3.147858110D-03 6.007968680D-07
-6.143397650D-11 2.599968870D-15                -6.268190300D+03-2.107446126D+02
H4F4            TPIS 1989 v1 pt1 p167; pt 2 p310.
 2 tpis89 H   4.00F   4.00    0.00    0.00    0.00 0   80.0253728   -1186932.336
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21654.080
 1.315109024D+05-1.840361560D+03 1.264093152D+01 2.495407360D-02-4.170394610D-05
 3.452523840D-08-1.072034360D-11 0.000000000D+00-1.364003454D+05-4.122913530D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21654.080
 3.354037990D+06-1.171922040D+04 2.765243565D+01-1.508934621D-03 2.257027572D-07
-1.744867255D-11 5.304351740D-16 0.000000000D+00-7.420213160D+04-1.388603332D+02
H5F5            TPIS 1989 v1 pt1 p168; pt 2 p311.
 2 tpis89 H   5.00F   5.00    0.00    0.00    0.00 0  100.0317160   -1490187.882
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        28045.138
 1.641361897D+05-2.300510396D+03 1.630140545D+01 3.119205422D-02-5.212926350D-05
 4.315611240D-08-1.340031413D-11 0.000000000D+00-1.714345408D+05-5.682157380D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        28045.138
 4.192290730D+06-1.464903043D+04 3.506554920D+01-1.886170471D-03 2.821289954D-07
-2.181090984D-11 6.630474160D-16 0.000000000D+00-9.368704200D+04-1.788592044D+02
H6F6            TPIS 1989 v1 pt1 p169; pt 2 p312.
 2 tpis89 H   6.00F   6.00    0.00    0.00    0.00 0  120.0380592   -1805545.131
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        34334.493
 1.956886618D+05-2.753909880D+03 1.975625055D+01 3.807717010D-02-6.341218880D-05
 5.219233290D-08-1.612185649D-11 0.000000000D+00-2.079269410D+05-7.113607980D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        34334.493
 5.024520320D+06-1.742817868D+04 4.214870500D+01-2.084564791D-03 2.930051519D-07
-2.052079159D-11 5.206937300D-16 0.000000000D+00-1.154497653D+05-2.163947001D+02
H7F7            TPIS 1989 v1 pt1 p170; pt 2 p313.
 2 tpis89 H   7.00F   7.00    0.00    0.00    0.00 0  140.0444024   -2099698.974
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        40827.254
 2.293867477D+05-3.220807860D+03 2.362235212D+01 4.366801880D-02-7.297990340D-05
 6.041786420D-08-1.876025627D-11 0.000000000D+00-2.418637479D+05-8.838812260D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        40827.254
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 5.868789830D+06-2.050863473D+04 4.989176110D+01-2.640634895D-03 3.949796330D-07
-3.053515088D-11 9.282601780D-16 0.000000000D+00-1.330177809D+05-2.592385142D+02
He              Ref-Elm. Moore NSRDS-NBS 35 1971; NSRDS-NBS 34 1970.
 3 g 5/97 HE  1.00    0.00    0.00    0.00    0.00 0    4.0026020          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 9.287239740D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 9.287239740D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.396845420D+06-2.194037652D+03 3.080231878D+00-8.068957550D-05 6.252784910D-09
-2.574990067D-13 4.429960218D-18                1.650518960D+04-4.048814390D+00
He+             Moore NSRDS-NBS 35 1971; NSRDS-NBS 34 1970. Cp/R=2.5
 3 g 3/97 HE  1.00E  -1.00    0.00    0.00    0.00 0    4.0020534    2378521.473
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.853233739D+05 1.621665557D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.853233739D+05 1.621665557D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.853233739D+05 1.621665557D+00
Hg              Hf:CODATA1989. Spec:NSRDS-NBS 35 vIII 1971 p191.
 3 g 1/98 HG  1.00    0.00    0.00    0.00    0.00 0  200.5900000      61380.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.636900080D+03 6.800201540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.146573510D+04-1.681269855D+02 2.718343098D+00-1.445026192D-04 5.158977660D-08
-9.472485010D-12 7.034797406D-16                7.688684930D+03 5.271236090D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.358443930D+08-4.433853810D+05 1.463223992D+02-2.318441669D-02 1.916335174D-06
-7.419662000D-11 1.067224054D-15                3.391999920D+06-1.201225990D+03
Hg+             NSRDS,NBS 35 vIII 1971 p196
 3 g 7/97 HG  1.00E  -1.00    0.00    0.00    0.00 0  200.5894514    1074643.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21                1.285037483D+05 7.493344500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.229984728D+04 2.732269908D+01 2.484182160D+00-4.426797610D-06 7.489685860D-09
-2.549887287D-12 2.819873366D-16                1.283188257D+05 7.625244570D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-5.498617710D+07 3.775543500D+04-7.155545550D+00 1.170310234D-03-7.931471440D-08
 4.029174000D-12-7.741071633D-17               -1.676894201D+05 9.116750020D+01
HgBr2
 2 J 3/62 HG  1.00BR  2.00    0.00    0.00    0.00 0  360.3980000     -85451.725
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.718892100D+00 2.578274300D-03-2.918023700D-06
 9.581844200D-10 1.387230700D-13               -1.237143400D+04-4.136708230D-01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.422699000D+00 7.868766300D-05-2.991030700D-08
 4.849822800D-12-2.793093300D-16               -1.252202000D+04-3.867339710D+00
I               Hf:CODATA1989. NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 3/97 I   1.00    0.00    0.00    0.00    0.00 0  126.9044700     106760.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.698199675D+02-2.716437233D+00 2.517385557D+00-5.730692070D-05 1.031716184D-07
-9.670641930D-11 3.706471651D-14                1.210750090D+04 7.405823130D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-7.785860570D+05 2.303279568D+03 2.886686091D-03 1.180878463D-03-2.264074866D-07
 1.963511339D-11-6.243525941D-16               -2.616792742D+03 2.558922997D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.747630780D+07-8.681111190D+04 3.950617020D+01-6.514063250D-03 5.380695340D-07
-1.969145066D-11 2.643177163D-16                6.384843030D+05-2.972997119D+02
I+              Spec: NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g10/97 I   1.00E  -1.00    0.00    0.00    0.00 0  126.9039214    1121351.028
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-8.014969010D+02 8.139052610D+00 2.470174760D+00 4.161393820D-05 7.133397860D-09
-7.105950140D-11 4.873766102D-14                1.340794213D+05 7.903420090D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
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-7.788385330D+05 2.404962651D+03-1.791751142D-01 1.227311979D-03-1.801494030D-07
 9.923983960D-12-9.775286439D-17              1.188531631D+05 2.710544347D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-6.314420010D+08 3.971131910D+05-9.860191990D+01 1.358236563D-02-9.920747650D-07
 3.684927700D-11-5.301687095D-16              -3.001474591D+06 8.790468740D+02
I-            JPCRD v14 n3 1985 p731.
 3 g10/97 I   1.00E   1.00    0.00    0.00    0.00 0  126.9050186    -194595.572
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.414970936D+04 6.113465380D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.414970936D+04 6.113465380D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.414970936D+04 6.113465380D+00
IF5           TPIS, v.1, pt.1,1989 p232-34.
 2 tpis89 I   1.00F   5.00    0.00    0.00    0.00 0  221.8964860    -841000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20044.142
 2.026113800D+05-3.598082730D+03 2.530294200D+01-1.348448360D-02 1.105458950D-05
-4.706217860D-09 7.859229090D-13              -8.700195430D+04-1.112689050D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20044.142
-3.621918460D+05-1.635362370D+02 1.612231540D+01-4.892667330D-05 1.080024220D-08
-1.236536050D-12 5.720823390D-17              -1.061667250D+05-5.398476130D+01
IF7           TPIS, v.1, pt.1,1989 p232,234-35.
 2 tpis89 I   1.00F   7.00    0.00    0.00    0.00 0  259.8932924    -961500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24123.333
 2.999669200D+05-5.501292290D+03 3.626989550D+01-2.095367880D-02 1.761391460D-05
-7.824847750D-09 1.404678520D-12              -9.331433310D+04-1.754135750D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24123.333
-5.614765950D+05-2.645406370D+02 2.219871710D+01-7.980865450D-05 1.768239830D-08
-2.031142670D-12 9.423845270D-17              -1.225251090D+05-8.773950160D+01
I2            TPIS 1989 v1 pt1 p220; pt2, p117.
 2 tpis89 I   2.00    0.00    0.00    0.00    0.00 0  253.8089400     62420.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10116.122
-5.087968770D+03-1.249585210D+01 4.504219090D+00 1.370962533D-04-1.390523014D-07
 1.174813853D-10-2.337541043D-14 0.000000000D+00 6.213469810D+03 5.583836940D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10116.122
-5.632594160D+06 1.793961560D+04-1.723055169D+01 1.244214080D-02-3.332768580D-06
 4.125477940D-10-1.960461713D-14 0.000000000D+00-1.068505292D+05 1.600531883D+02
In            Hf:TPIS96;ARK FUR FYSIK V34 1966 p578;NSRDS-NBS35 1971
 3 g 1/99 IN  1.00    0.00    0.00    0.00    0.00 0  114.8180000    240700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6198.649
 5.149518050D+04-9.177999020D+02 8.938687950D+00-2.224112602D-02 3.823881940D-05
-2.890116948D-08 8.047481221D-12              3.239031620D+04-2.764567028D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6198.649
-1.683608899D+06 2.210473186D+03 3.472219370D+00-1.082267422D-03 3.479699980D-07
-5.158092410D-11 3.183043089D-15              1.095965206D+04 2.557189088D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6198.649
-2.289146601D+06 3.908691060D+04-1.789204885D+01 3.655375250D-03-2.576493626D-07
 7.929188320D-12-9.066642170D-17              -2.376257502D+05 1.738048645D+02
In+           IP:Arkiv fur Fysik v34n46p577;Levels:NSRDS-NBS35 1971
 3 g 4/99 IN  1.00E  -1.00    0.00    0.00    0.00 0  114.8174514      6996.425
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.150488908D-01-2.523854672D-03 2.500011877D+00-2.869063919D-08 3.753870400D-11
-2.525942419D-14 6.842932660D-18              9.610930170D+01 5.963254400D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.536995140D+04-1.445142103D+02 2.681812441D+00-1.157480060D-04 3.947714810D-08
-6.879243620D-12 4.819204920D-16              1.004261440D+03 4.683759180D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-6.188028020D+07 1.322640301D+04 7.453303840D+00-1.893250634D-03 2.114636410D-07
-8.432019810D-12 1.185570972D-16              -1.335858982D+05-2.765870435D+01
InBr          Hsubl(cr),Props:TPIS 1996 pt1 p289 p291;pt2 p233
 2 tpis96 IN  1.00BR  1.00    0.00    0.00    0.00 0  194.7220000     -54115.879
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10084.121
-2.540851435D+03-5.294704710D+01 4.717438090D+00-4.344669490D-04 6.513513640D-07
-4.403995150D-10 1.234046209D-13              -7.607594280D+03 4.258881000D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10084.121
 7.948374420D+05-2.318183711D+03 7.032889580D+00-1.245920568D-03 3.276693350D-07
-3.003771106D-11 5.853192770D-16              6.957627290D+03-1.273502660D+01
InBr2         D0,cons: TPIS 1996 pt1 p292; pt2 p234.
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 2 tpis96 IN  1.00BR  2.00    0.00    0.00    0.00 0  274.6260000    -149729.059
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14424.341
-6.619878900D+01-2.365897310D+02 7.926545160D+00-1.994547959D-03 2.420414153D-06
-1.548924922D-09 4.058148390D-13              -1.895355588D+04-5.338867540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14424.341
-3.217162030D+05 4.792682100D+02 7.102649480D+00-5.514019780D-04 3.157862421D-07
-5.511254510D-11 3.172161390D-15              -2.370923659D+04 1.193263347D-01
InBr3            Subl,cons: TPIS 1996 pt1 p292-4; pt2 p236.
 2 tpis96 IN  1.00BR  3.00    0.00    0.00    0.00 0  354.5300000    -256587.267
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19912.733
-4.990115300D+03-2.805930452D+02 1.110356060D+01-2.379995808D-03 2.887825281D-06
-1.844500707D-09 4.814395870D-13              -3.250504910D+04-1.871748987D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19912.733
-3.505783100D+04-4.858721320D+00 1.000406131D+01-1.767620958D-06 4.164016060D-10
-5.015528870D-14 2.415414123D-18              -3.393179240D+04-1.229069868D+01
InCL             D0,props: TPIS 1996 pt1 p281, pt2 p225
 2 tpis96 IN  1.00CL  1.00    0.00    0.00    0.00 0  150.2707000     -72147.883
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9752.117
 6.430713030D+03-2.178267726D+02 5.418830900D+00-2.048005100D-03 2.702295936D-06
-1.795319798D-09 4.847469090D-13              -8.959841070D+03-1.203002248D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9752.117
-2.745751636D+05 8.940986910D+02 3.268118390D+00 9.180277780D-04-3.083262431D-07
 5.745458810D-11-3.645275750D-15              -1.561603430D+04 1.266880075D+01
InCL2            D0,cons: TPIS 1996 pt1 p283; pt2 p226.
 2 tpis96 IN  1.00CL  2.00    0.00    0.00    0.00 0  185.7234000    -201483.416
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13956.384
 9.935164870D+03-4.172101860D+02 8.588494910D+00-3.348385610D-03 3.997866640D-06
-2.525301853D-09 6.544490330D-13              -2.426480269D+04-1.164522210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13956.384
-3.328719840D+05 4.757691610D+02 7.105443690D+00-5.525786960D-04 3.160567738D-07
-5.514453680D-11 3.173680380D-15              -2.995095917D+04-2.294560357D+00
InCL3            Subl,cons: TPIS 1996 pt1 p284-6; pt2 p228.
 2 tpis96 IN  1.00CL  3.00    0.00    0.00    0.00 0  221.1761000    -369693.227
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18306.773
 2.614743044D+04-8.414604560D+02 1.311784790D+01-6.435282470D-03 7.554874750D-06
-4.705078560D-09 1.204213663D-12              -4.326469580D+04-3.500081550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18306.773
-7.114043630D+04-1.628425068D+01 1.001309622D+01-5.544528880D-06 1.279877732D-09
-1.518261505D-13 7.226562770D-18              -4.758974170D+04-1.669761621D+01
InF              D0,props: TPIS 1996 pt1 p272, pt2 p217.
 2 tpis96 IN  1.00F   1.00    0.00    0.00    0.00 0  133.8164032    -193419.989
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9217.111
 3.190123320D+04-5.295254260D+02 6.172886260D+00-2.986035832D-03 3.233778030D-06
-1.856975575D-09 4.465024970D-13              -2.187176282D+04-7.591216620D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9217.111
-4.689001200D+05 1.321019051D+03 2.881329353D+00 1.041591078D-03-3.090754867D-07
 4.926646560D-11-2.699156425D-15              -3.308369810D+04 1.396688303D+01
InF2             D0,cons: TPIS 1996 pt1 p274; pt2 p218.
 2 tpis96 IN  1.00F   2.00    0.00    0.00    0.00 0  152.8148064    -457186.824
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12588.776
 7.522480210D+04-1.088616881D+03 9.481705210D+00-2.893229367D-03 1.516224649D-06
-7.989517810D-11-1.466781026D-13              -5.124336150D+04-2.146666090D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12588.776
 4.318960340D+05-1.688472420D+03 8.925863010D+00-1.049188835D-03 2.723934190D-07
-2.882959902D-11 1.073493779D-15              -4.673691940D+04-1.932464363D+01
InF3             Hsubl,Cons: TPIS 1996 pt1 p276; pt2 p220.
 2 tpis96 IN  1.00F   3.00    0.00    0.00    0.00 0  171.8132096    -863079.566
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16320.434
 1.071608336D+05-1.660071901D+03 1.395972813D+01-5.018693260D-03 3.226367530D-06
-7.823385970D-10-3.726999800D-14              -9.795214990D+04-4.606353470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16320.434
-1.656855506D+05-7.965889290D+01 1.005913347D+01-2.350816639D-05 5.163512930D-09
-5.888048810D-13 2.715090697D-17              -1.068682627D+05-2.132968218D+01
InH              D0,props: TPIS 1996 pt1 p269, pt2 p215
 2 tpis96 IN  1.00H   1.00    0.00    0.00    0.00 0  115.8259400     215016.904
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8684.104
-5.152828720D+04 7.813792590D+02-8.433385340D-01 1.044471274D-02-9.761074820D-06
 4.540635200D-09-8.169906900D-13               2.110048908D+04 2.939346222D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8684.104
 7.797406660D+05-3.646882080D+03 9.542967350D+00-3.481281720D-03 1.304805603D-06
-2.182950701D-10 1.274009748D-14               4.643295460D+04-3.659329230D+01
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InI             D0,props: TPIS 1996 pt1 p298, pt2 p241.
 2 tpis96 IN  1.00I   1.00    0.00    0.00    0.00 0  241.7224700     26417.124
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10271.124
-4.686348740D+02-5.685530990D+01 4.781849690D+00-6.619368310D-04 1.027666742D-06
-7.270592070D-10 2.077991102D-13                2.095570254D+03 4.885515130D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10271.124
 1.529221772D+06-4.690373680D+03 1.004593462D+01-3.140434110D-03 9.460834390D-07
-1.253862848D-10 5.949805640D-15                3.152478143D+04-3.297697490D+01
InI2            D0,cons: TPIS 1996 pt1 p300; pt2 p243.
 2 tpis96 IN  1.00I   2.00    0.00    0.00    0.00 0  368.6269400    -39460.643
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14912.757
-4.513890600D+03-1.183726870D+02 7.473110080D+00-1.034474090D-03 1.271465534D-06
-8.227820300D-10 2.178307019D-13               -6.278536040D+03-6.667297500D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14912.757
-3.130671665D+05 4.813810700D+02 7.100914180D+00-5.506559920D-04 3.156120735D-07
-5.509170540D-11 3.171162830D-15               -1.043012750D+04 2.141662307D+00
InI3            Subl,cons: TPIS 1996 pt1 p301-3; pt2 p245.
 2 tpis96 IN  1.00I   3.00    0.00    0.00    0.00 0  495.5314100   -105435.914
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20852.086
-8.728397170D+03-1.265914859D+02 1.050659120D+01-1.106109314D-03 1.354335766D-06
-8.709453460D-10 2.285186350D-13               -1.508269063D+04-1.211411745D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20852.086
-2.196742567D+04-2.151167521D+00 1.000182200D+01-8.002214700D-07 1.897343164D-10
-2.296252460D-14 1.109838196D-18               -1.572406335D+04-9.170888690D+00
InO             D0,props: TPIS 1996 pt1 p261, pt2 p212
 2 tpis96 IN  1.00O   1.00    0.00    0.00    0.00 0  130.8174000    145993.109
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9042.109
-1.154727169D+05 1.753668703D+03-6.965033810D+00 2.961698958D-02-3.123332334D-05
 1.437244720D-08-2.235519898D-12                8.188679590D+03 6.608621260D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9042.109
-8.052130950D+05 1.693064203D+03 4.760863580D+00-7.340718400D-04 3.229597760D-07
-4.580150380D-11 1.954611725D-15                4.005519810D+03 3.500742460D+00
InOH            Hf0,cons: TPIS 1996 pt1 p271; pt2 p216.
 2 tpis96 IN  1.00O   1.00H   1.00    0.00    0.00 0  131.8253400   -124447.344
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10736.839
 6.123463020D+04-1.195863129D+03 1.041427981D+01-6.870002500D-03 6.214128780D-06
-2.408203181D-09 3.177641780D-13               -1.079852170D+04-3.189890840D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10736.839
 8.525128930D+05-2.350317172D+03 7.984515140D+00 9.915815620D-05-6.212385450D-08
 1.016169575D-11-5.682557640D-16               -1.536213610D+03-2.043107643D+01
In2Br2          Hf0,constants: Gurvich TPIS 1996 pt1 p294; pt2 p237.
 2 tpis96 IN  2.00BR  2.00    0.00    0.00    0.00 0  389.4440000   -196305.215
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21434.943
-9.221188300D+03-3.616677030D+01 1.014728771D+01-3.255775200D-04 4.022327480D-07
-2.604080237D-10 6.867689550D-14               -2.644883479D+04-1.000360073D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21434.943
-1.290781804D+04-6.075401240D-01 1.000052163D+01-2.312058331D-07 5.517315720D-11
-6.708620190D-15 3.253841650D-19               -2.663136878D+04-9.149949470D+00
In2Br4          D0,cons: TPIS 1996 pt1 p295; pt2 p238.
 2 tpis96 IN  2.00BR  4.00    0.00    0.00    0.00 0  549.2520000   -436508.683
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31798.117
-1.425555379D+04-2.866009341D+02 1.713866292D+01-2.473506655D-03 3.017273071D-06
-1.934900430D-09 5.065874250D-13               -5.593753060D+04-3.837105980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31798.117
-4.453463710D+04-4.911523980D+00 1.600413764D+01-1.810579975D-06 4.281715740D-10
-5.171998020D-14 2.496142837D-18               -5.739175410D+04-3.174906390D+01
In2Br6          Hf0,cons: TPIS 1996 pt1 p296; pt2 p239.
 2 tpis96 IN  2.00BR  6.00    0.00    0.00    0.00 0  709.0600000   -628683.430
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       43096.728
-1.758940752D+04-4.859034480D+02 2.391654505D+01-4.142061490D-03 5.033849320D-06
-3.219103650D-09 8.410220070D-13               -7.988844460D+04-6.437871880D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       43096.728
-6.945039480D+04-8.402368170D+00 2.200703884D+01-3.068251799D-06 7.235965730D-10
-8.722870580D-14 4.203469910D-18               -8.235759850D+04-5.322192800D+01
In2CL2          Hf0,cons: TPIS 1996 pt1 p287; pt2 p229.
 2 tpis96 IN  2.00CL  2.00    0.00    0.00    0.00 0  300.5414000   -232177.375
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20223.895
-1.142848747D+04-1.416015827D+02 1.056853314D+01-1.244253440D-03 1.526076784D-06
-9.826402810D-10 2.580766990D-13               -3.026327087D+04-1.565105259D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20223.895
-2.616606332D+04-2.401955489D+00 1.000203984D+01-8.975190030D-07 2.130755553D-10
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-2.581140900D-14 1.248404822D-18              -3.098016735D+04-1.234946804D+01
In2CL4          Hf0,cons: TPIS 1996 pt1 p287; pt2 p230.
 2 tpis96 IN  2.00CL  4.00    0.00    0.00    0.00 0  371.4468000    -579125.856
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       29456.525
 9.814083080D+03-8.488959010D+02 1.923410360D+01-6.815674240D-03 8.129220730D-06
-5.125076850D-09 1.324324755D-12              -7.027688140D+04-5.582666180D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       29456.525
-8.503771790D+04-1.552464614D+01 1.601269668D+01-5.441549870D-06 1.267594997D-09
-1.514110365D-13 7.245404540D-18              -7.461921740D+04-3.691151100D+01
In2CL6          Hf0,cons: TPIS 1996 pt1 p288; pt2 p231.
 2 tpis96 IN  2.00CL  6.00    0.00    0.00    0.00 0  442.3522000    -882340.029
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38423.462
 3.004663159D+04-1.585621359D+03 2.796489470D+01-1.245506052D-02 1.475341213D-05
-9.252689200D-09 2.381233885D-12              -1.048828300D+05-9.788405250D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38423.462
-1.499400484D+05-2.988680816D+01 2.202425362D+01-1.033652301D-05 2.397911922D-09
-2.855307516D-13 1.363051661D-17              -1.130110233D+05-6.293986290D+01
In2F2           D0,cons: Gurvich TPIS 1996 pt1 p276; pt2 p221.
 2 tpis96 IN  2.00F   2.00    0.00    0.00    0.00 0  267.6328064    -532234.300
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18039.900
 7.255717100D+03-6.448265650D+02 1.247539512D+01-5.246089620D-03 6.283616210D-06
-3.974342340D-09 1.029559356D-12              -6.384892450D+04-3.108004586D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18039.900
-6.409715440D+04-1.163740672D+01 1.000956511D+01-4.114086910D-06 9.608828320D-10
-1.150013486D-13 5.511437480D-18              -6.714277850D+04-1.661718474D+01
In2F4           D0,cons: TPIS 1996 pt1 p277; pt2 p222.
 2 tpis96 IN  2.00F   4.00    0.00    0.00    0.00 0  305.6296128   -1284788.126
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24763.074
 1.225213611D+05-2.444998374D+03 2.342425457D+01-1.291427120D-02 1.308700476D-05
-7.181673930D-09 1.648386404D-12              -1.466942111D+05-8.943560050D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24763.074
-2.205977486D+05-7.822083770D+01 1.605923872D+01-2.394023240D-05 5.329582790D-09
-6.144609570D-13 2.859099598D-17              -1.595716347D+05-4.469574580D+01
In2F6           Hf298,cons: TPIS 1996 pt1 p279; pt2 p223.
 2 tpis96 IN  2.00F   6.00    0.00    0.00    0.00 0  343.6264192   -1960000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33567.102
 1.825490583D+05-3.552111710D+03 3.275425230D+01-1.868064635D-02 1.892443162D-05
-1.038916311D-08 2.386637271D-12              -2.239648760D+05-1.363626758D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33567.102
-3.170966380D+05-1.167440973D+02 2.208847456D+01-3.577733930D-05 7.968959040D-09
-9.191681700D-13 4.278494150D-17              -2.426661118D+05-7.155328560D+01
In2I2           D0,cons: Gurvich TPIS 1996 pt1 p303; pt2 p246.
 2 tpis96 IN  2.00I   2.00    0.00    0.00    0.00 0  483.4449400     -27813.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22058.476
-6.681925010D+03-1.449103222D+01 1.005929122D+01-1.314921486D-04 1.628373589D-07
-1.056087811D-10 2.788963879D-14              -6.279602600D+03-7.291130980D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22058.476
-8.148157300D+03-2.444544443D-01 1.000021086D+01-9.376789250D-08 2.242988180D-11
-2.732299303D-15 1.327135699D-19              -6.352651500D+03-6.947725420D+00
In2I4           Hf0,cons: TPIS 1996 pt1 p304; pt2 p247.
 2 tpis96 IN  2.00I   4.00    0.00    0.00    0.00 0  737.2538800    -199143.181
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33468.979
-1.501028064D+04-9.744797900D+01 1.639383950D+01-8.659380210D-04 1.065671801D-06
-6.879252680D-10 1.810240886D-13              -2.830388443D+04-2.986294828D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33468.979
-2.505699251D+04-1.642155234D+00 1.600140149D+01-6.187066280D-07 1.472308565D-10
-1.786593333D-14 8.652338780D-19              -2.879655333D+04-2.757790375D+01
In2I6           Hf0,cons: TPIS 1996 pt1 p305; pt2 p248.
 2 tpis96 IN  2.00I   6.00    0.00    0.00    0.00 0  991.0628200    -319720.040
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       45088.120
-2.232640607D+04-2.000786874D+02 2.280417927D+01-1.761331313D-03 2.161510393D-06
-1.392400447D-09 3.658171880D-13              -4.412547680D+04-5.273802030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       45088.120
-4.311905850D+04-3.390350590D+00 2.200288128D+01-1.268348706D-06 3.012121900D-10
-3.649676710D-14 1.765530622D-18              -4.513820270D+04-4.806868370D+01
In2O            Hf0,cons: TPIS 1996 pt1 p264; pt2 p213.
 2 tpis96 IN  2.00O   1.00    0.00    0.00    0.00 0  245.6354000     -34763.707
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12796.504
 5.065653500D+04-8.070363670D+02 8.642067270D+00-1.533035446D-03 2.866419382D-07
 4.981134970D-10-2.554320291D-13              -1.924908459D+03-1.490718759D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12796.504
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-9.232786360D+04-5.201127280D+01 7.038723620D+00-1.543821179D-05 3.399700870D-09
-3.885457100D-13 1.795125270D-17              -6.270926800D+03-4.421820410D+00
K              Hf: CODATA 89. Spec: JPCRD v14 sup2 1985 p11.
 3 g 7/97 K   1.00    0.00    0.00    0.00    0.00 0   39.0983000     89000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 9.665143930D+00-1.458059455D-01 2.500865861D+00-2.601219276D-06 4.187306580D-09
-3.439722110D-12 1.131569009D-15              9.959493490D+03 5.035822260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-3.566422360D+06 1.085289825D+04-1.054134898D+01 8.009801350D-03-2.696681041D-06
 4.715294150D-10-2.976897350D-14              -5.875337010D+04 9.738551240D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 9.205786590D+08-6.935300280D+05 1.911270788D+02-2.305931672D-02 1.430294866D-06
-4.409335020D-11 5.366769166D-16              5.395082190D+06-1.622158805D+03
K+             JPCRD v14 sup2 1985 p26.
 3 g 6/97 K   1.00E  -1.00    0.00    0.00    0.00 0   39.0977514    514007.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              6.107516860D+04 4.347404440D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              6.107516860D+04 4.347404440D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.177901245D+07-1.415076630D+04 6.248954270D+00-5.187436800D-04 3.959640680D-08
-1.584335542D-12 2.603558905D-17              1.722753576D+05-2.781728990D+01
K-             JPCRD v14 n3 1985 p731.
 3 g 9/97 K   1.00E   1.00    0.00    0.00    0.00 0   39.0988486     34418.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              3.394150710D+03 4.347446530D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              3.394150710D+03 4.347446530D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              3.394150710D+03 4.347446530D+00
KBO2
 2 J 6/71 K   1.00B   1.00O   2.00    0.00    0.00 0   81.9081000    -674054.737
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.396780100D+00 1.216920200D-02-1.180421800D-05
 5.131655100D-09-6.593272000D-13              -8.282701200D+04 7.573243100D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.550250800D+00 2.566182300D-03-1.067156600D-06
 1.985188500D-10-1.370416800D-14              -8.365383400D+04-8.492700000D+00
KCN
 2 J 3/66 K   1.00C   1.00N   1.00    0.00    0.00 0   65.1157400     79499.339
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.081071100D+00 5.526595600D-03-9.115712100D-06
 8.448881700D-09-3.005154800D-12              7.866216100D+03 1.863330464D-01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.800712000D+00 1.720078600D-03-7.079107400D-07
 1.319924700D-10-9.190832300D-15              7.727262800D+03-3.158848012D+00
KCL
 2 J 3/66 K   1.00CL  1.00    0.00    0.00    0.00 0   74.5510000    -214685.057
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.990856900D+00 2.108916900D-03-3.183653000D-06
 2.252530800D-09-5.909417900D-13              -2.708018400D+04 5.512004450D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.463673300D+00 1.222920700D-04-9.171921000D-09
 9.264824200D-13-1.040791700D-17              -2.717313300D+04 3.248089950D+00
KF
 2 J 6/69 K   1.00F   1.00    0.00    0.00    0.00 0   58.0967032    -326776.265
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.515606600D+00 3.786842200D-03-5.586499500D-06
 3.775143800D-09-9.392421800D-13              -4.047607900D+04 6.313385450D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.404070000D+00 1.783372500D-04-3.609379700D-08
 5.883958700D-12-3.469404600D-16              -4.065588900D+04 2.031095850D+00
KF2-
 2 J12/68 K   1.00F   2.00E   1.00    0.00    0.00 0   77.0956550    -694556.675
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.250757300D+00 8.638371800D-03-1.340367300D-05
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 9.414083200D-09-2.468260200D-12              -8.538397100D+04-4.772247130D-01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.258163800D+00 2.670355700D-04-1.138463000D-07
 2.140768500D-11-1.482707000D-15              -8.578083900D+04-1.010327830D+01
KH
 2 J 3/63 K   1.00H   1.00    0.00    0.00    0.00 0   40.1062400     123012.034
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.815775600D+00 3.987106000D-03-3.341054800D-06
 8.860294200D-10 1.140284700D-13              1.380583800D+04 6.725178990D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.960338600D+00 7.219032300D-04-2.691871500D-07
 5.261730000D-11-3.787268300D-15              1.350183700D+04 8.553450830D-01
KO
 2 J12/67 K   1.00O   1.00    0.00    0.00    0.00 0   55.0977000      71131.606
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.741077800D+00 3.124201700D-03-4.802003900D-06
 3.466060500D-09-9.359979100D-13              7.336871400D+03 6.566923890D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.424477800D+00 1.993615500D-04-3.712883700D-08
 7.130830000D-12-5.036968700D-16              7.205233100D+03 3.307668490D+00
KO-
 2 J12/67 K   1.00O   1.00E   1.00    0.00    0.00 0   55.0982486    -138073.651
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.708366000D+00 3.237648000D-03-4.969050000D-06
 3.572884600D-09-9.608026800D-13             -1.781860700D+04 5.316625880D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.420108400D+00 2.012426600D-04-3.933099600D-08
 7.559851100D-12-5.344227500D-16             -1.795610900D+04 1.920004080D+00
KOH             JPCRD v26 n4 1997 p1031.
 2 g 9/97 K   1.00O   1.00H   1.00    0.00    0.00 0   56.1056400    -232000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11674.650
 1.770684196D+04-6.153205220D+02 8.684075720D+00-3.962849510D-03 3.408650590D-06
-9.601972220D-10 8.494054970D-15             -2.677903261D+04-2.174495666D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11674.650
 8.917271950D+05-2.334179072D+03 7.972578710D+00 1.038863156D-04-6.315893470D-08
 1.027938106D-11-5.736685820D-16             -1.443696469D+04-2.076401416D+01
KOH+
 2 J12/71 K   1.00O   1.00H   1.00E  -1.00    0.00 0   56.1050914     497913.829
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.432516700D+00 8.463162500D-03-1.424785500D-05
 1.110662500D-08-3.156361200D-12              5.829263200D+04 2.873345730D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.680614000D+00 1.212095100D-03-3.344711700D-07
 4.172793200D-11-1.879391300D-15              5.816760200D+04-2.554151370D+00
K2              JANAF tabulated data.
 2 j12/83 K   2.00    0.00    0.00    0.00    0.00 0   78.1966000     123672.129
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10738.129
 1.950025530D+04-3.962524140D+02 7.480306370D+00-1.107868240D-02 2.251546960D-05
-2.102644850D-08 6.843817470D-12              1.529890140D+04-1.133351920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10738.129
-4.205896420D+06 1.170570910D+04-5.492380230D+00 2.862953000D-03-5.696245250D-07
 5.949128510D-11-2.541736430D-15             -6.272919630D+04 8.055174320D+01
K2C2N2
 2 J 3/66 K   2.00C   2.00N   2.00    0.00    0.00 0  130.2314800      -8365.237
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.113305800D+01 1.151636200D-02-1.947653300D-05
 1.816985900D-08-6.464725200D-12             -4.698069300D+03-2.126797292D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.262575400D+01 3.412399600D-03-1.403488800D-06
 2.615639600D-10-1.820686500D-14             -4.975361400D+03-2.815390492D+01
K2CL2
 2 J 3/66 K   2.00CL  2.00    0.00    0.00    0.00 0  149.1020000    -617657.012
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.706797400D+00 6.015404700D-03-1.130393900D-05
 9.662081400D-09-3.105565700D-12             -7.706769600D+04-8.537547250D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.904106900D+00 1.117970700D-04-5.039119700D-08
 9.993461400D-12-7.270300900D-16             -7.727233000D+04-1.409028200D+01
K2F2
 2 J 6/69 K   2.00F   2.00    0.00    0.00    0.00 0  116.1934064    -862757.408
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
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 0.000000000D+00 0.000000000D+00 7.832950400D+00 8.924083100D-03-1.471985200D-05
 1.098246900D-08-3.072172000D-12              -1.063875200D+05-8.242382810D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.814809600D+00 2.045308100D-04-8.707166500D-08
 1.633722700D-11-1.128725600D-15              -1.067598700D+05-1.764180300D+01
K2O2H2          JPCRD v26 n4 1997 p1031.
 2 g 9/97 K   2.00O   2.00H   2.00    0.00    0.00 0  112.2112800    -641000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22384.933
 8.174788370D+03-1.130630680D+03 1.815303256D+01-7.737431080D-03 6.837614010D-06
-2.054691111D-09 7.672877510D-14              -7.574965170D+04-6.391759470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22384.933
 1.773523196D+06-4.665292470D+03 1.694308128D+01 2.085297143D-04-1.264714762D-07
 2.057506565D-11-1.148042134D-15              -5.051263310D+04-6.334773920D+01
K2SO4
 2 J 6/78 K   2.00S   1.00O   4.00    0.00    0.00 0  174.2602000   -1094144.144
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.475852000D+00 4.877323700D-02-6.842008000D-05
 4.688631600D-08-1.272108200D-11              -1.342808500D+05 1.234482860D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.537410800D+01 4.105613900D-03-1.814893500D-06
 3.549724300D-10-2.555875400D-14              -1.369532900D+05-4.614381540D+01
Kr              Ref-Elm. Spec:JPCRD v20 n5 1991 p859.
 3 g 8/97 KR  1.00    0.00    0.00    0.00    0.00 0   83.8000000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02 5.490956510D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.643639057D+02-7.910050820D-01 2.500920585D+00-5.328164110D-07 1.620730161D-10
-2.467898017D-14 1.478585040D-18              -7.403488940D+02 5.484398150D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.375531087D+09 9.064030530D+05-2.403481435D+02 3.378312030D-02-2.563103877D-06
 9.969787790D-11-1.521249677D-15              -7.111667370D+06 2.086866326D+03
Kr+             Levels:JPCRD v20 n5 1991 p859.
 3 g 7/97 KR  1.00E  -1.00    0.00    0.00    0.00 0   83.7994514    1356953.918
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-5.650402860D+03 6.930740810D+01 2.157028132D+00 8.711228930D-04-1.181609730D-06
 7.862198630D-10-1.832589387D-13              1.621164118D+05 8.818242260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.216567015D+05 1.166167840D+03 4.869655320D-01 1.429223599D-03-3.949628610D-07
 4.982853510D-11-2.406719258D-15              1.556002861D+05 2.059230986D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-3.319875960D+07 1.797953100D+04-7.155015940D-01 2.671088984D-04-6.196251880D-09
-4.107025960D-13 2.000619351D-17              1.648114259D+04 3.620325750D+01
Li              Hf:CODATA1989. NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 7/97 LI  1.00    0.00    0.00    0.00    0.00 0    6.9410000    159300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.841390197D+04 2.447622965D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.125610652D+06-3.463536730D+03 6.566611920D+00-2.260983356D-03 5.922289160D-07
-6.281635100D-11 2.884948238D-15              4.034637400D+04-2.655918195D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.604352623D+09-1.521952201D+06 3.454400500D+02-3.779674850D-02 2.222420069D-06
-6.691570800D-11 8.088023606D-16              1.217791847D+07-3.006680193D+03
Li+             Cp/R=2.5. IP: Moore, NSRDS-NBS 35 v1 1971
 3 g 3/97 LI  1.00E  -1.00    0.00    0.00    0.00 0    6.9404514    685719.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               8.172724550D+04 1.754357228D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               8.172724550D+04 1.754357228D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               8.172724550D+04 1.754357228D+00
Li-             JPCRD v14 n3 1985 p731.
 3 g 1/98 LI  1.00E   1.00    0.00    0.00    0.00 0    6.9415486     93474.728
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.049698659D+04 1.754594332D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
```

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 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.049698659D+04 1.754594332D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.049698659D+04 1.754594332D+00
LiALF4
 2 J12/79 LI  1.00AL  1.00F   4.00    0.00    0.00 0  109.9161508   -1853531.697
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.540342100D+00 5.198588100D-02-8.618803100D-05
 6.749681600D-08-2.036750900D-11                -2.253576700D+05 1.257193199D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.403774200D+01 2.248264200D-03-1.001000200D-06
 1.967024900D-10-1.420888600D-14                -2.276275700D+05-4.236014801D+01
LiBO2
 2 J 6/71 LI  1.00B   1.00O   2.00    0.00    0.00 0   49.7508000    -646856.749
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.743547400D+00 1.447525700D-02-1.520968800D-05
 7.413654100D-09-1.224219100D-12                -7.943775600D+04 8.012025640D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.426609600D+00 2.704375700D-03-1.128474100D-06
 2.106239800D-10-1.458490900D-14                -8.037028500D+04-1.060079180D+01
LiCL
 2 J 6/62 LI  1.00CL  1.00    0.00    0.00    0.00 0   42.3937000    -195712.165
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.990690600D+00 5.033864200D-03-6.567197900D-06
 3.805016000D-09-7.611745500D-13                -2.460318200D+04 7.328184480D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.271214300D+00 3.140029100D-04-1.012313000D-07
 1.845185300D-11-1.239873100D-15                -2.488444200D+04 1.041721580D+00
LiF
 2 J12/68 LI  1.00F   1.00    0.00    0.00    0.00 0   25.9394032    -340794.847
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.852886900D+00 3.953278100D-03-3.172498500D-06
 4.324439700D-10 3.705566700D-13                -4.198726500D+04 6.791028870D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.043024800D+00 5.704105400D-04-2.145414400D-07
 4.060901300D-11-2.835792000D-15                -4.229931800D+04 6.976954670D-01
LiFO
 2 J 9/65 LI  1.00F   1.00O   1.00    0.00    0.00 0   41.9388032     -92041.760
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.500179000D+00 1.266171700D-02-1.415758900D-05
 6.450637400D-09-7.426143100D-13                -1.226553400D+04 1.214401820D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.992610900D+00 1.113920000D-03-4.788849300D-07
 9.106833200D-11-6.384912300D-15                -1.310098900D+04-5.336603290D+00
LiF2-
 2 J12/68 LI  1.00F   2.00E   1.00    0.00    0.00 0   44.9383550    -711293.506
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.471813600D+00 1.063671300D-02-1.177764600D-05
 5.676548700D-09-8.465984000D-13                -8.696311100D+04 5.140927950D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.344859000D+00 1.257127200D-03-5.352283000D-07
 1.011302500D-10-7.058174400D-15                -8.766789000D+04-9.298402850D+00
LiH
 2 J 9/67 LI  1.00H   1.00    0.00    0.00    0.00 0    7.9489400     140625.945
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.420948600D+00-6.806736600D-04 5.652738100D-06
-6.218034800D-09 2.153175500D-12                1.588494500D+04 1.065741940D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.588429700D+00 1.072769100D-03-4.019458800D-07
 7.382855700D-11-4.926964400D-15                1.571762500D+04-3.750389650D-01
LiN
 2 J12/66 LI  1.00N   1.00    0.00    0.00    0.00 0   20.9477400     334730.691
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.889430000D+00 5.221253400D-03-6.596902100D-06
 3.728899700D-09-7.235514300D-13                3.921632300D+04 7.288871450D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.225807700D+00 3.966718700D-04-1.249399300D-07
 2.317475900D-11-1.585191700D-15                3.891695200D+04 7.008514810D-01
LiO
 2 J 3/64 LI  1.00O   1.00    0.00    0.00    0.00 0   22.9404000      84098.280
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   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.838900700D+00 5.153862600D-03-6.308238200D-06
 3.411438500D-09-6.163134300D-13              9.088431400D+03 7.913117890D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.187620500D+00 4.118657400D-04-1.452029600D-07
 2.725307000D-11-1.886477500D-15              8.779525900D+03 1.231425990D+00
LiO-
 2 J12/67 LI  1.00O   1.00E   1.00    0.00    0.00 0   22.9409486    -66943.828
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.851586600D+00 5.016988000D-03-5.954747500D-06
 3.039945100D-09-4.787296900D-13             -9.077807600D+03 6.459470670D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.181021700D+00 4.178500000D-04-1.502484500D-07
 2.839773200D-11-1.978918100D-15             -9.384970200D+03-1.423923370D-01
LiOH            JPCRD v25 n4,1996 p1211.
 2 g12/96 LI  1.00O   1.00H   1.00    0.00    0.00 0   23.9483400    -229000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11336.961
 4.573917250D+03-1.030912117D+02 4.272388090D+00 8.465269500D-03-1.386155567D-05
 1.101104878D-08-3.291263060D-12             -2.848730645D+04-8.774661430D-01
  1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11336.961
 8.500669210D+05-2.430519740D+03 8.055293810D+00 6.896706920D-05-5.527474390D-08
 9.368402810D-12-5.313965360D-16             -1.365908112D+04-2.457582930D+01
LiOH+
 2 J12/71 LI  1.00O   1.00H   1.00E  -1.00    0.00 0   23.9477914     778249.755
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.637973900D+00 1.089715400D-02-1.722967000D-05
 1.266792700D-08-3.416525900D-12              9.216119300D+04 3.637760920D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.532926900D+00 1.377793100D-03-4.065930900D-07
 5.559091000D-11-2.860462400D-15              9.188857900D+04-4.993592680D+00
LiON
 2 J 9/66 LI  1.00O   1.00N   1.00    0.00    0.00 0   36.9471400     179918.898
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.670116400D+00 7.256817700D-03-5.868114600D-06
 1.162831200D-09 4.270412200D-13              2.027170300D+04 6.682495110D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.812349600D+00 1.287062600D-03-5.466771000D-07
 1.031498700D-10-7.193044700D-15              1.969230200D+04-4.344705590D+00
Li2             JANAF tabulated data.
 2 J12/83 LI  2.00    0.00    0.00    0.00    0.00 0   13.8820000     215900.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       9675.116
 6.778486550D+03-2.246206590D+02 5.296037870D+00-1.272413250D-03 1.205845590D-06
-9.818685630D-11-2.416698380D-13              2.573638220D+04-6.869259970D+00
  1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       9675.116
 3.767645250D+07-1.185747130D+05 1.482167740D+02-8.378531870D-02 2.424919740D-05
-3.275820160D-09 1.652000040D-13              7.723071660D+05-1.021697260D+03
Li2CL2
 2 J 6/62 LI  2.00CL  2.00    0.00    0.00    0.00 0   84.7874000    -598521.423
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.280135100D+00 1.838410000D-02-2.876944800D-05
 2.031335900D-08-5.343324700D-12             -7.416000300D+04 2.792794220D-01
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.524561400D+00 5.245883400D-04-2.233794900D-07
 4.195111400D-11-2.902130600D-15             -7.499026300D+04-2.003167160D+01
Li2F2
 2 J12/68 LI  2.00F   2.00    0.00    0.00    0.00 0   51.8788064    -942791.003
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.400750800D+00 2.706623700D-02-3.925618000D-05
 2.572259900D-08-6.223722500D-12             -1.150109100D+05 1.089177880D+01
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.956663600D+00 1.171926900D-03-5.099050400D-07
 9.791753400D-11-6.921560200D-15             -1.163722800D+05-2.088633120D+01
Li2O
 2 J 3/64 LI  2.00O   1.00    0.00    0.00    0.00 0   29.8814000    -166935.467
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.972170800D+00 9.246092100D-03-9.359614900D-06
 3.463916000D-09-7.565888000D-14             -2.159698800D+04 2.552304090D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.619874800D+00 9.687944800D-04-4.149050600D-07
 7.863733700D-11-5.496929200D-15             -2.225532500D+04-1.082155900D+01
Li2O2
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 2 J 3/64 LI  2.00O   2.00    0.00    0.00    0.00 0   45.8808000    -242656.425
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.537523200D+00 1.734422300D-02-2.719797100D-05
 1.930562900D-08-5.120795700D-12              -3.140204400D+04-2.768312910D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.527526000D+00 5.302101300D-04-2.300586200D-07
 4.403083100D-11-3.101870200D-15              -3.218248400D+04-2.185911200D+01
Li2O2H2          JPCRD v25 n4,1996 p1211.
 2 g12/96 LI  2.00O   2.00H   2.00    0.00    0.00 0   47.8966800    -737000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15579.040
 1.894419736D+05-2.779126941D+03 1.530240424D+01 1.070722542D-02-2.510051911D-05
 2.224893730D-08-6.949312090D-12              -7.702772460D+04-6.514147350D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15579.040
 1.215363488D+06-3.982020720D+03 1.585873681D+01 7.509330590D-04-2.585266977D-07
 3.646906280D-11-1.904173044D-15              -6.738772230D+04-6.647181550D+01
Li2SO4
 2 J12/78 LI  2.00S   1.00O   4.00    0.00    0.00 0  109.9456000   -1041842.051
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.114572500D-01 5.945117900D-02-8.636349000D-05
 6.117108700D-08-1.709892300D-11              -1.275084200D+05 2.038032790D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.492959500D+01 4.609747400D-03-2.037955600D-06
 3.986257900D-10-2.870303000D-14              -1.306352800D+05-4.916649110D+01
Li3CL3
 2 J 6/62 LI  3.00CL  3.00    0.00    0.00    0.00 0  127.1811000   -1004679.135
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.574595900D+00 3.974923900D-02-5.650821300D-05
 3.629414500D-08-8.578470000D-12              -1.235335100D+05 4.680596580D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.431944000D+01 1.885400700D-03-8.197833000D-07
 1.573549400D-10-1.111947200D-14              -1.255885100D+05-4.271102260D+01
Li3F3
 2 J12/68 LI  3.00F   3.00    0.00    0.00    0.00 0   77.8182096   -1517221.026
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.641397500D+00 3.987869600D-02-5.724899100D-05
 3.719354400D-08-8.923012500D-12              -1.851985200D+05 2.162359670D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.436442200D+01 1.828549800D-03-7.922115900D-07
 1.515452900D-10-1.067567300D-14              -1.872373600D+05-4.506091300D+01
Mg               Hf:CODATA 1989. Spec:JPCRD v20 n1 1991 p83-152.
 3 g 6/97 MG  1.00    0.00    0.00    0.00    0.00 0   24.3050000     147100.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.694658761D+04 3.634330140D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-5.364831550D+05 1.973709576D+03-3.633776900D-01 2.071795561D-03-7.738051720D-07
 1.359277788D-10-7.766898397D-15              4.829188110D+03 2.339104998D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.166012586D+09-1.008355665D+06 1.619680021D+02-8.790130350D-03-1.925690961D-08
 1.725045214D-11-4.234946112D-16              8.349525900D+06-1.469355261D+03
Mg+              Spec:JPCRD v20 n1 1991 p97.
 3 g 6/97 MG  1.00E  -1.00    0.00    0.00    0.00 0   24.3044514     891047.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.064223354D+05 4.327443460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.914758821D+04 4.877347920D+01 2.457662661D+00 1.218104674D-05 1.897261686D-09
-1.580433756D-12 2.135732238D-16              1.061022394D+05 4.646442860D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.015949550D+08-2.281591735D+05 5.421745710D+01-5.983017190D-03 3.657189130D-07
-1.020737688D-11 1.024202854D-16              1.932463961D+06-4.480157830D+02
MgBr             Props & D0: TPIS 1996 pt1 p417, pt2 p331.
 2 tpis96 MG  1.00BR  1.00    0.00    0.00    0.00 0  104.2090000       6163.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9588.115
 7.361419140D+03-2.395789881D+02 5.360560420D+00-1.667141829D-03 1.981137765D-06
-1.201637202D-09 3.032148099D-13              5.915634440D+02-1.421771179D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9588.115
 2.477604216D+04-6.417687520D+02 6.019932090D+00-1.391004302D-03 6.443330960D-07
-1.197734078D-10 7.421644240D-15              2.824060334D+03-6.264439920D+00
MgBr2            Hsubl & cons: TPIS v3 pt1 p420; pt2 p333.
 2 tpis96 MG  1.00BR  2.00    0.00    0.00    0.00 0  184.1130000    -306743.219
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14757.281
 2.148477999D+04-5.154528900D+02 9.273258750D+00-3.470049040D-03 3.921840790D-06
-2.377174864D-09 5.967025560D-13              -3.652443850D+04-1.791077763D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14757.281
-4.326899010D+04-1.283036001D+01 7.510024300D+00-4.152332400D-06 9.426499180D-10
-1.103873928D-13 5.201104310D-18              -3.919886020D+04-7.409168030D+00
MgCL            Props & D0: TPIS 1996 pt1 p412, pt2 p328.
 2 tpis96 MG  1.00CL  1.00    0.00    0.00    0.00 0   59.7577000     -54704.887
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9363.113
 2.043995280D+04-4.072155160D+02 5.880372300D+00-2.594175042D-03 2.945953528D-06
-1.750648628D-09 4.337959330D-13              -5.851444950D+03-6.023553280D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9363.113
 1.041328453D+06-3.380158330D+03 8.637775470D+00-2.447789643D-03 7.841969440D-07
-1.126409380D-10 5.810620730D-15               1.327188977D+04-2.703803148D+01
MgCL+
 2 J 6/68 MG  1.00CL  1.00E  -1.00    0.00    0.00 0   59.7571514     652722.898
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.601223000D+00 3.479185900D-03-5.135314300D-06
 3.444633700D-09-8.384820600D-13               7.731468800D+04 6.133859330D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.351234400D+00-3.796719000D-03 2.471294500D-06
-5.082365300D-10 3.367262500D-14               7.648087900D+04-8.290362270D+00
MgCLF
 2 J 3/66 MG  1.00CL  1.00F   1.00    0.00    0.00 0   78.7561032    -569024.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.157042930D+00 1.645347900D-02-3.011268690D-05
 2.579746060D-08-8.424875470D-12              -6.989100400D+04 1.022554020D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.570822520D+00 4.488762080D-04-1.779948190D-07
 3.063182050D-11-1.915545440D-15              -7.052359770D+04-5.835554140D+00
MgCL2           Hsubl & cons: TPIS v3 pt1 p416; pt2 p330.
 2 tpis96 MG  1.00CL  2.00    0.00    0.00    0.00 0   95.2104000    -399169.896
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13900.604
 3.637824680D+04-7.307844960D+02 9.661030510D+00-3.660212940D-03 3.610819350D-06
-1.928769286D-09 4.309912350D-13              -4.646914570D+04-2.360113219D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13900.604
-6.835217010D+04-2.490899393D+01 7.518783200D+00-7.564518260D-06 1.679293770D-09
-1.931706275D-13 8.971657820D-18              -5.032686910D+04-1.053269327D+01
MgF             Props & D0: TPIS 1996 pt1 p408, pt2 p325.
 2 tpis96 MG  1.00F   1.00    0.00    0.00    0.00 0   43.3034032    -232266.792
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8969.108
 3.823001620D+04-4.803310390D+02 5.068468940D+00 5.212029300D-04-1.874026347D-06
 1.759241129D-09-5.609403190D-13              -2.659114296D+04-3.768969210D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8969.108
-1.695883782D+05 3.588757630D+02 3.936001650D+00 4.813044140D-04-1.658385409D-07
 3.336052290D-11-2.270104205D-15              -3.169323990D+04 4.410565900D+00
MgF+
 2 J12/75 MG  1.00F   1.00E  -1.00    0.00    0.00 0   43.3028546     512303.557
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.438765400D+00 2.225265400D-03-5.462120200D-06
 1.408427600D-08-8.072690600D-12               6.051566600D+04 5.778354560D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.368105700D+00 4.117596600D-03-2.939479700D-06
 7.271184300D-10-5.984480200D-14               5.953600000D+04-1.345777940D+00
MgF2            Hsub(0),Cons: TPIS v3 pt1 p411; pt2 p327.
 2 tpis96 MG  1.00F   2.00    0.00    0.00    0.00 0   62.3018064    -735498.060
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12622.440
 4.338429550D+04-6.616511770D+02 7.453448520D+00 3.520814050D-03-6.955764580D-06
 5.619923480D-09-1.688028906D-12              -8.687183670D+04-1.545476790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12622.440
-1.244419584D+05-8.687343750D+01 7.563581230D+00-2.499267978D-05 5.440129140D-09
-6.158245760D-13 2.822792666D-17              -9.060019440D+04-1.420796990D+01
MgF2+
 2 J12/75 MG  1.00F   2.00E  -1.00    0.00    0.00 0   62.3012578     591997.228
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.521288400D+00 1.526955600D-02-2.518008900D-05
 1.963549900D-08-5.905491900D-12               6.965838800D+04 7.390209450D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.891067300D+00 7.178128300D-04-3.294117200D-07
 6.588112800D-11-4.587322800D-15               6.899314500D+04-8.713013950D+00
MgH             Props & D0: TPIS 1996 pt1 p401, pt2 p320.
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 2 tpis96 MG  1.00H   1.00    0.00    0.00    0.00 0   25.3129400     229786.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8682.104
-4.958679150D+04 7.500278650D+02-6.442047500D-01 9.826301010D-03-8.789822440D-06
 3.823353520D-09-6.003725760D-13                2.302279383D+04 2.657165344D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8682.104
-1.005748598D+05 1.952890106D+03-1.317191549D+00 5.603665800D-03-2.137334980D-06
 3.324880500D-10-1.824672746D-14                1.598582755D+04 3.431233160D+01
MgI             D0,Props: TPIS 1996 pt1 p420, pt2 p334.
 2 tpis96 MG  1.00I   1.00    0.00    0.00    0.00 0  151.2094700      61206.317
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9741.117
 2.943889099D+03-1.690248574D+02 5.147251830D+00-1.321186997D-03 1.623056505D-06
-1.005114222D-09 2.567337785D-13                6.845890270D+03 8.593132250D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9741.117
-2.370562811D+06 6.916452480D+03-3.183894490D+00 4.051551140D-03-9.774290750D-07
 1.023329400D-10-3.790304870D-15               -3.818551110D+04 5.993104380D+01
MgI2            Hsubl & cons: TPIS v3 pt1 p423; pt2 p336.
 2 tpis96 MG  1.00I   2.00    0.00    0.00    0.00 0  278.1139400    -171706.029
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15294.471
 1.594739709D+04-4.160412720D+02 9.010638320D+00-3.090359024D-03 3.621264260D-06
-2.260138392D-09 5.809055550D-13               -2.080441400D+04-1.412175736D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15294.471
-3.340299180D+04-9.343511780D+00 7.507468540D+00-3.147707890D-06 7.241336470D-10
-8.567664950D-14 4.069691700D-18               -2.294555505D+04-5.241272590D+00
MgN
 2 J 3/64 MG  1.00N   1.00    0.00    0.00    0.00 0   38.3117400     288691.678
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.889454900D+00 5.175717500D-03-6.584901600D-06
 3.721893300D-09-7.230596400D-13                3.368105800D+04 9.297589460D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.221441700D+00 3.648924000D-04-1.299573000D-07
 2.441894000D-11-1.691775900D-15                3.338293100D+04 2.732051960D+00
MgO             D0,Props: TPIS 1996 pt1 p398, pt2 p318.
 3 tpis96 MG  1.00O   1.00    0.00    0.00    0.00 0   40.3044000      32261.307
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8909.107
 3.513659740D+05-5.287197160D+03 3.382060060D+01-8.400489630D-02 1.210016160D-04
-7.630795020D-08 1.701022862D-11                2.790679519D+04-1.624886199D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8909.107
-1.586738367D+07 3.420468100D+04-1.774087677D+01 7.004963050D-03-1.104138249D-06
 8.957488530D-11-3.052513649D-15               -2.300504434D+05 1.738984472D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8909.107
 2.290059050D+06-2.073499632D+04 1.444150005D+01-1.490609900D-03 1.052119343D-07
-3.523030610D-12 4.613111760D-17                1.490218815D+05-8.007281730D+01
MgOH            Hf0 & cons: TPIS v3 pt1 p404; pt2 p322.
 2 tpis96 MG  1.00O   1.00H   1.00    0.00    0.00 0   41.3123400    -132428.980
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11124.284
 3.839851620D+04-7.367383640D+02 7.920664460D+00-5.950940590D-04-2.112941162D-06
 3.228282110D-09-1.214159329D-12               -1.392326188D+04-1.916078109D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11124.284
 6.648664750D+05-1.770750355D+03 7.269999270D+00 5.336842760D-04-1.980894443D-07
 3.025677088D-11-1.554849476D-15               -6.149114560D+03-1.671027009D+01
MgOH+
 2 J12/75 MG  1.00O   1.00H   1.00E  -1.00    0.00 0   41.3117914     584436.764
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.783142100D+00 1.922852700D-02-3.350314300D-05
 2.749136400D-08-8.515100700D-12                6.915058400D+04 1.193052360D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.282447900D+00 1.664043700D-03-5.401665100D-07
 8.346782400D-11-5.003616800D-15                6.859581600D+04-4.150388630D+00
Mg(OH)2         Hf0 & cons: TPIS v3 pt1 p407; pt2 p324.
 2 tpis96 MG  1.00O   2.00H   2.00    0.00    0.00 0   58.3196800    -551995.808
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17131.558
 5.245894670D+04-1.289056383D+03 1.389327642D+01-7.806693670D-04-4.151257230D-06
 6.109473040D-09-2.274138833D-12               -6.295089150D+04-5.015353340D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17131.558
 1.713709254D+06-4.730005350D+03 1.448925967D+01 1.907819857D-04-1.226834131D-07
 2.015343753D-11-1.128993279D-15               -3.887724670D+04-5.840498120D+01
MgS             Props & D0: TPIS 1996 pt1 p425, pt2 p338.
 2 tpis96 MG  1.00S   1.00    0.00    0.00    0.00 0   56.3710000     120649.311
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9234.111
-9.565788090D+03 1.443637798D+02 1.813794717D+00 1.147168775D-02-2.220170412D-05
 1.995344981D-08-6.090688740D-12                1.276501517D+04 1.461335754D+01
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9234.111
 2.650794328D+07-7.711355860D+04 8.463771680D+01-3.644250680D-02 8.403084420D-06
-9.539882170D-10 4.264658030D-14                5.078931170D+05-5.834655830D+02
Mg2             Props and D0: TPIS 1996 pt1 p393 pt2 p316.
 2 tpis96 MG  2.00    0.00    0.00    0.00    0.00 0   48.6100000     286513.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9542.115
 4.545195590D+03 4.115850040D+02 4.841196170D-01 4.891969650D-03-6.395536840D-06
 4.299764550D-09-1.164624418D-12                3.181641790D+04 2.640432143D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9542.115
 3.038224994D+04 5.945240460D+01 2.352706666D+00 1.378537924D-04-5.895692040D-08
 1.104045317D-11-6.558868290D-16                3.351036560D+04 1.588177377D+01
Mg2F4
 2 J12/75 MG  2.00F   4.00    0.00    0.00    0.00 0  124.6036128   -1718408.746
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.229905300D+00 4.929084900D-02-8.644967200D-05
 7.045937100D-08-2.188711000D-11               -2.094929900D+05 5.003236150D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.467201600D+01 1.529931800D-03-6.834711700D-07
 1.346046900D-10-9.738339800D-15               -2.114376600D+05-4.427824400D+01
Mn              Hf:JPCRD v16 n1 1987 p97. Levels:JPCRD v14 sup2 1985.
 3 g 7/97 MN  1.00    0.00    0.00    0.00    0.00 0   54.9380490     282400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.034061359D-01-1.551537349D-03 2.500009148D+00-2.723162066D-08 4.333897430D-11
-3.511093890D-14 1.136032201D-17                3.321935190D+04 6.649325463D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.855155820D+03 8.838588440D+02-3.648662580D-02 2.703720687D-03-1.324971998D-06
 2.872603290D-10-1.923633570D-14                2.867803487D+04 2.292541198D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.936189040D+09-2.353549748D+06 5.377244800D+02-5.824812570D-02 3.330475100D-06
-9.689631050D-11 1.133286034D-15                1.879530161D+07-4.690097890D+03
Mn+             JPCRD v14 sup2 1985.
 3 g 6/97 MN  1.00E  -1.00    0.00    0.00    0.00 0   54.9375004    1005871.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.458017700D+02-4.251151330D+00 2.521281028D+00-5.565087280D-05 8.037162210D-08
-6.093550970D-11 1.900014268D-14                1.202533602D+05 6.683468162D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 6.471314100D+05-2.403796253D+03 5.937715750D+00-2.341014594D-03 7.464165640D-07
-9.075969730D-11 4.467879847D-15                1.349902108D+05-1.702666341D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.717119921D+09-9.029185830D+05 1.784788847D+02-1.566770206D-02 7.346534410D-07
-1.750673350D-11 1.667889239D-16                7.443546080D+06-1.568005804D+03
Mo              Hf:JPCRD v16 n1 1987 p107.Levels:JPCRD v17 n1 1988 p155.
 3 g 7/97 MO  1.00    0.00    0.00    0.00    0.00 0   95.9400000     658500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 7.646367910D+01-1.159269043D+00 2.506929462D+00-2.099249725D-05 3.414779430D-08
-2.841269591D-11 9.492443321D-15                7.845899800D+04 7.601835660D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.573271000D+06-1.662365811D+04 2.135147077D+01-1.003069377D-02 2.409784357D-06
-1.811267352D-10 1.034189087D-15                1.842646473D+05-1.275326434D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 6.205038910D+09-3.855961600D+06 9.371595060D+02-1.108164544D-01 6.929123900D-06
-2.199865715D-10 2.798315513D-15                3.062163602D+07-8.122811340D+03
Mo+             JPCRD v17 n1 1988 p155.
 3 g 7/97 MO  1.00E  -1.00    0.00    0.00    0.00 0   95.9394514    1349012.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.298236623D+02-1.560279908D+00 2.507600281D+00-1.923789063D-05 2.673316651D-08
-1.937174292D-11 5.729735412D-15                1.615103759D+05 7.442543460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.298891120D+07-3.948276230D+04 4.866599780D+01-2.605352326D-02 7.215431920D-06
-8.719164960D-10 3.788423040D-14                4.118948570D+05-3.216791030D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.731253943D+09 8.776685240D+05-1.669716753D+02 1.732439603D-02-9.372726850D-07
 2.593422324D-11-2.913787941D-16               -6.989098130D+06 1.517101780D+03
Mo-             JPCRD v14 n3 1985 p731.
 3 g10/97 MO  1.00E   1.00    0.00    0.00    0.00 0   95.9405486     580324.628
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.905123690D+04 7.485659540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.905123690D+04 7.485659540D+00
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   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.905123690D+04 7.485659540D+00
MoO3
 2 TPIS82 MO  1.00O   3.00    0.00    0.00    0.00 0  143.9382000    -364414.339
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.654312100D+00 1.449099200D-02-7.668139000D-06
-6.098464000D-09 5.182580900D-12               -4.548309400D+04 8.505218890D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.559907900D+00 1.513690700D-03-6.137326000D-07
 1.075889000D-10-6.227755500D-15               -4.676527000D+04-1.670282500D+01
Mo2O6
 2 TPIS82 MO  2.00O   6.00    0.00    0.00    0.00 0  287.8764000   -1149456.646
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.754672100D+00 3.262506400D-02-1.665990600D-05
-1.503960000D-08 1.236035800D-11               -1.418333800D+05-6.450927310D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.392333200D+01 1.290874900D-02-7.392938600D-06
 1.745410900D-09-1.441066800D-13               -1.429283100D+05-3.644861400D+01
Mo3O9
 2 TPIS82 MO  3.00O   9.00    0.00    0.00    0.00 0  431.8146000   -1902048.676
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.357742400D+01 4.538931000D-02-2.130595400D-05
-2.286776600D-08 1.775232700D-11               -2.345968800D+05-2.857713900D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.226229900D+01 1.858496700D-02-1.058935700D-05
 2.492675200D-09-2.054253600D-13               -2.362003800D+05-7.108818600D+01
Mo4O12
 2 TPIS82 MO  4.00O  12.00    0.00    0.00    0.00 0  575.7528000   -2625550.231
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.872747800D+01 6.115949900D-02-2.914191300D-05
-3.065805000D-08 2.401182000D-11               -3.237659400D+05-5.008838400D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.043174700D+01 2.473264600D-02-1.411854900D-05
 3.327129200D-09-2.743901600D-13               -3.259036300D+05-1.072803370D+02
Mo5O15
 2 TPIS82 MO  5.00O  15.00    0.00    0.00    0.00 0  719.6910000   -3329138.617
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.388705400D+01 7.614100000D-02-3.517472900D-05
-3.986486500D-08 3.063112300D-11               -4.105210600D+05-7.160417700D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.862254300D+01 3.074274200D-02-1.753604700D-05
 4.130623000D-09-3.405577100D-13               -4.132415600D+05-1.437367570D+02
N              Hf:CODATA1989. Spec:NSRDS-NBS 3 sec5 1975.
 3 g 5/97 N   1.00    0.00    0.00    0.00    0.00 0   14.0067400    472680.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                5.610463780D+04 4.193909320D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 8.876501380D+04-1.071231500D+02 2.362188287D+00 2.916720081D-04-1.729515100D-07
 4.012657880D-11-2.677227571D-15                5.697351330D+04 4.865235790D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.475181050D+08-3.107574980D+05 6.916782740D+01-6.847988130D-03 3.827572400D-07
-1.098367709D-11 1.277986024D-16                2.550585618D+06-5.848769710D+02
N+             NSRDS-NBS 3 sec5 1975.
 3 g 6/97 N   1.00E  -1.00    0.00    0.00    0.00 0   14.0061914    1882127.624
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7116.524
 5.237079210D+03 2.299958315D+00 2.487488821D+00 2.737490756D-05-3.134447576D-08
 1.850111332D-11-4.447350984D-15                2.256284738D+05 5.076835070D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7116.524
 2.904970374D+05-8.557908610D+02 3.477389290D+00-5.288267190D-04 1.352350307D-07
-1.389834122D-11 5.046166279D-16                2.310809984D+05-1.994142261D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7116.524
 1.646092148D+07-1.113165218D+04 4.976986640D+00-2.005393583D-04 1.022481356D-08
-2.691430863D-13 3.539931593D-18                3.136284696D+05-1.706645952D+01
N-             EA:JPCRD v14 n3 1985 p731. Spec:JANAF 1985 12/82.
 3 j12/82 N   1.00E   1.00    0.00    0.00    0.00 0   14.0072886    473537.545
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6498.345
 1.428934638D+03 7.520687090D+00 2.475858824D+00 4.415023460D-05-4.657766010D-08
 2.638862446D-11-6.213819110D-15                5.617531660D+04 5.150502820D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6498.345
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 2.051106014D+03 1.635387404D+00 2.497936299D+00 1.273470155D-06-3.965632200D-10
 5.954259630D-14-3.415843300D-18                5.620590040D+04 5.019432790D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6498.345
 2.199831428D+03 7.682241210D-01 2.499511240D+00 1.351807305D-07-1.818981536D-11
 1.108192493D-15-2.419223446D-20                5.621092380D+04 5.008716500D+00
NCO             Hf0: JCP,v99,1993 p4638. Cons: JPCRD v27 n2,1988 p269.
 2 g 2/96 N   1.00C   1.00O   1.00    0.00    0.00 0   42.0168400     131843.928
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10194.932
 9.507969170D+03-1.957329856D+02 4.235127910D+00 3.903719150D-03 3.855140120D-07
-2.853519565D-09 1.234513806D-12                1.556962567D+04 2.042503416D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10194.932
 7.392929780D+04-1.617258377D+03 8.574919530D+00-3.764554980D-04 7.038295860D-08
-6.686532180D-12 2.988934173D-16                2.289407064D+04-2.552768024D+01
ND
 2 J 6/77 N   1.00D   1.00    0.00    0.00    0.00 0   16.0208420     375309.257
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.720648800D+00-1.534184800D-03 3.187742600D-06
-1.509140100D-09 9.712611400D-14                4.407275600D+04 1.649556720D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.829703400D+00 1.658417500D-03-6.328733300D-07
 1.147768500D-10-7.831858400D-15                4.425595100D+04 6.006628820D+00
ND2
 2 J 6/77 N   1.00D   2.00    0.00    0.00    0.00 0   18.0349440     185353.401
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.026978000D+00-1.408512800D-03 7.776581500D-06
-6.496757500D-09 1.755417000D-12                2.109802800D+04 1.754842950D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.351539100D+00 3.376316200D-03-1.321345700D-06
 2.680067900D-10-2.081017400D-14                2.107774900D+04 4.373879750D+00
ND3
 2 J 6/77 N   1.00D   3.00    0.00    0.00    0.00 0   20.0490460     -58576.719
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.942783900D+00 5.103529100D-03 2.739282100D-06
-4.684766200D-09 1.627667400D-12               -8.165156300D+03 6.155220380D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.196156600D+00 6.731175800D-03-2.642340000D-06
 4.763086800D-10-3.280482800D-14               -8.396652700D+03 4.162907180D+00
NF              TPIS 1989 v1 pt1 p372;pt2 p234. Data:TPIS 1978 pt2 p243.
 2 tpis89 N   1.00F   1.00    0.00    0.00    0.00 0   33.0051432     232990.500
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8738.105
-3.504927750D+04 6.674502990D+02-1.201665982D+00 1.452074253D-02-1.822873148D-05
 1.160136864D-08-2.973416333D-12                2.395414002D+04 3.089260613D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8738.105
 8.002987330D+05-3.237696580D+03 8.703408870D+00-2.701025798D-03 9.150042110D-07
-1.365256630D-10 7.234624410D-15                4.642819450D+04-3.019933066D+01
NF2             TPIS 1989 v1 pt1 p373. NASA RP1271 1992 METHOD NRRAO1
 2 g 4/99 N   1.00F   2.00    0.00    0.00    0.00 0   52.0035464      34421.447
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10581.605
 1.511831104D+04 9.196389940D+01 4.947301790D-01 2.001847323D-02-2.767712684D-05
 1.872924867D-08-5.020318040D-12                2.839279606D+03 2.270515785D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10581.605
-1.945010078D+05-3.536034070D+02 7.263494360D+00-8.402380400D-05 2.326721111D-08
-2.667577562D-12 1.236070614D-16                3.435440590D+03-1.336102396D+01
NF3             TPIS 1989 v1 pt1 p375. NASA RP1271 1992 METHOD NRRAO2.
 2 g 4/99 N   1.00F   3.00    0.00    0.00    0.00 0   71.0019496    -131700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11854.511
 8.757149280D+04-9.031832890D+02 4.027417270D+00 2.314439555D-02-3.415106470D-05
 2.409483651D-08-6.633464190D-12               -1.237232074D+04 3.026439163D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11854.511
-3.496268760D+05-4.973728670D+02 1.036866128D+01 8.900687650D-05 5.882654360D-08
-3.157737664D-12 1.714329953D-16               -1.713183352D+04-3.098920773D+01
NH              Props: TPIS 1978 v1 pt2 p223 DelH: JPC 1989 v93 p530.
 3 g 4/99 N   1.00H   1.00    0.00    0.00    0.00 0   15.0146800     357032.001
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8601.103
 1.359651320D+04-1.900296604D+02 4.518496790D+00-2.432776899D-03 2.377587464D-06
-2.592797084D-10-2.659680792D-13                4.280972190D+04-3.886557620D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8601.103
 1.958141991D+06-5.782861300D+03 9.335742020D+00-2.292910311D-03 6.076092480D-07
-6.647942750D-11 2.384234783D-15                7.898912340D+04-4.116970000D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8601.103
 9.524636790D+07-8.585826910D+04 2.980445181D+01-2.979563697D-03 1.656334158D-07
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-4.744791840D-12 5.570148290D-17              6.961434270D+05-2.229027379D+02
NH+             Props: TPIS 1989 v1 pt2 p216. Hf:JCP 1985 v83 p4319.
 3 g 5/99 N   1.00H   1.00E  -1.00    0.00    0.00 0   15.0141314    1665787.914
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9495.114
 4.253656850D+03-2.458222206D+02 6.708919490D+00-1.038489430D-02 1.509008623D-05
-9.580512190D-09 2.333206758D-12              2.001077797D+05-1.395057232D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9495.114
 1.405709438D+06-4.136215710D+03 7.632014480D+00-1.228325778D-03 2.721187746D-07
-2.010098289D-11 3.717190180D-17              2.258975960D+05-2.786784834D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9495.114
 2.392941759D+08-1.741658624D+05 5.107907910D+01-5.567623700D-03 3.273391600D-07
-9.797978060D-12 1.186543279D-16              1.554705305D+06-4.065968920D+02
NHF             TPIS 1989 v1 pt1 p386; pt2 p247.
 2 tpis89 N   1.00H   1.00F   1.00    0.00    0.00 0   34.0130832     112000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10029.728
-5.110686660D+04 9.612292200D+02-2.706464740D+00 2.036567210D-02-2.425564940D-05
 1.551557030D-08-4.058469010D-12              7.909610910D+03 4.099327570D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10029.728
 9.013857120D+05-3.463387780D+03 8.705798490D+00-4.018946180D-04 2.322764160D-08
 6.280460140D-12-6.283060730D-16              3.337059030D+04-2.900478530D+01
NHF2            TPIS 1989 v1 pt1 p388; pt2 p249.
 2 tpis89 N   1.00H   1.00F   2.00    0.00    0.00 0   53.0114864    -103000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10807.439
-5.626200090D+04 1.205768160D+03-6.017588710D+00 3.760042490D-02-4.619217840D-05
 2.942488030D-08-7.598763990D-12             -1.897020020D+04 5.901748540D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10807.439
 7.393975160D+05-4.004384660D+03 1.221312670D+01-6.969908920D-04 1.270923150D-07
-1.246923200D-11 5.085333750D-16              9.133638460D+03-4.867774600D+01
NH2             TPIS 1989. JPCRD v17 n2 1988 p282. JPC v93 1989 p530.
 2 g 5/99 N   1.00H   2.00    0.00    0.00    0.00 0   16.0226200     189134.662
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9937.815
-3.115971998D+04 4.750670790D+02 1.374616245D+00 6.299342450D-03-5.975903790D-06
 4.482282550D-09-1.410400817D-12              1.929106785D+04 1.538923094D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9937.815
 1.669007546D+06-5.610379470D+03 9.971875030D+00-1.178276343D-03 4.233947770D-07
-6.539740680D-11 3.619860350D-15              5.689057760D+04-4.379353410D+01
NH2F            TPIS 1989 v1 pt1 p387; pt2 p248.
 2 tpis89 N   1.00H   2.00F   1.00    0.00    0.00 0   35.0210232     -75000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10104.976
-1.092374760D+05 1.844919780D+03-7.673871600D+00 3.229533440D-02-3.388108670D-05
 1.971871550D-08-4.810205150D-12             -1.878318960D+04 6.861483910D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10104.976
 1.927205340D+06-7.500447160D+03 1.395589580D+01-1.184804420D-03 2.050678670D-07
-1.908761310D-11 7.389236210D-16              3.552927340D+04-6.731185320D+01
NH3             TPIS 1989 p219. JRNBS 1968 v72A p207 for low T.
 2 tpis89 N   1.00H   3.00    0.00    0.00    0.00 0   17.0305600     -45940.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10043.121
-7.681226150D+04 1.270951578D+03-3.893229130D+00 2.145988418D-02-2.183766703D-05
 1.317385706D-08-3.332322060D-12             -1.264886413D+04 4.366014940D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10043.121
 2.452389535D+06-8.040894240D+03 1.271346201D+01-3.980186580D-04 3.552502750D-08
 2.530923570D-12-3.322700530D-16              4.386191960D+04-6.462330250D+01
NH4+            Hf0,Cons: TPIS 1989 v1 pt1 p355; pt2 p220.
 2 tpis89 N   1.00H   4.00E  -1.00    0.00    0.00 0   18.0379514     644904.945
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9978.772
-2.668315752D+05 3.763020690D+03-1.571327725D+01 4.548820210D-02-4.379962120D-05
 2.464478293D-08-5.961532330D-12 0.000000000D+00 5.823284720D+04 1.112087189D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9978.772
 4.141889000D+06-1.442072042D+04 2.011893564D+01-1.971492619D-03 3.112721421D-07
-2.602979969D-11 8.894342130D-16 0.000000000D+00 1.664196236D+05-1.201535728D+02
NO              D0,Props: TPIS 1978,1989 v1 pt1 p326; pt2 p203.
 3 tpis89 N   1.00O   1.00    0.00    0.00    0.00 0   30.0061400      91271.310
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9179.110
-1.143916503D+04 1.536467592D+02 3.431468730D+00-2.668592368D-03 8.481399120D-06
-7.685111050D-09 2.386797655D-12              9.098214410D+03 6.728727490D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9179.110
 2.239018716D+05-1.289651623D+03 5.433936030D+00-3.656034900D-04 9.880966450D-08
-1.416076856D-11 9.380184620D-16              1.750317656D+04-8.501667090D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9179.110
-9.575303540D+08 5.912434480D+05-1.384566826D+02 1.694339403D-02-1.007351096D-06
 2.912584076D-11-3.295109350D-16             -4.677501240D+06 1.242081218D+03
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NO+             Cp,S,IP(NO): TPIS 1989 v1 pt1 p330;pt2 p205.
 3 tpis89 N   1.00O   1.00E  -1.00    0.00    0.00 0   30.0055914    990809.704
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8670.104
 1.398106635D+03-1.590446941D+02 5.122895400D+00-6.394388620D-03 1.123918342D-05
-7.988581260D-09 2.107383677D-12                1.187495132D+05-4.398431810D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8670.104
 6.069876900D+05-2.278395427D+03 6.080324670D+00-6.066847580D-04 1.432002611D-07
-1.747990522D-11 8.935014060D-16                1.322709615D+05-1.519879837D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8670.104
 2.676400347D+09-1.832948690D+06 5.099249390D+02-7.113819280D-02 5.317659880D-06
-1.963208212D-10 2.805268230D-15                1.443308939D+07-4.324044460D+03
NOCL            TPIS 1989 v1 pt1 p389. NASA RP1271 1992 METHOD PANDK.
 2 g 4/99 N   1.00O   1.00CL  1.00    0.00    0.00 0   65.4588400      52698.828
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11364.488
 2.308835209D+04-5.495983840D+02 7.730463360D+00-5.073910900D-03 1.062996184D-05
-8.793249700D-09 2.648180166D-12                7.389898390D+03-1.318393617D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11364.488
-6.133413330D+05-3.919298830D+02 9.138917220D+00-2.605664613D-03 1.295687247D-06
-2.215378352D-10 1.280394898D-14                4.517328420D+03-2.307323931D+01
NOF             TPIS 1989 v1 pt1 p382. NASA RP1271 1992.
 2 g 4/99 N   1.00O   1.00F   1.00    0.00    0.00 0   49.0045432     -65000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10720.271
 4.755024260D+04-7.253904170D+02 7.213996360D+00-2.532427181D-03 6.377743900D-06
-5.518305880D-09 1.681935713D-12               -5.609722520D+03-1.289663494D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10720.271
 1.889069274D+06-6.731022660D+03 1.419018767D+01-3.693124620D-03 9.938575140D-07
-1.080748188D-10 4.210354430D-15                3.209900780D+04-6.370266840D+01
NOF3            TPIS 1989 v1 pt1 p385; pt2 p246.
 2 tpis89 N   1.00O   1.00F   3.00    0.00    0.00 0   87.0013496    -187000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13697.653
 1.488406470D+05-2.241115760D+03 1.302391560D+01 5.462962870D-03-8.640377440D-06
 5.912563580D-09-1.576691880D-12               -1.328310940D+04-4.877523830D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13697.653
-2.786218940D+05-1.252171250D+03 1.390810210D+01-3.566065800D-04 7.783682840D-08
-8.849156490D-12 4.075616880D-16               -2.025749850D+04-5.106777720D+01
NO2             Hf0,Cons: TPIS 1989 v1 pt1 p332; pt2 p207.
 2 g 4/99 N   1.00O   2.00    0.00    0.00    0.00 0   46.0055400      34193.019
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10208.175
-5.642038780D+04 9.633085720D+02-2.434510974D+00 1.927760886D-02-1.874559328D-05
 9.145497730D-09-1.777647635D-12               -1.547925037D+03 4.067851340D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10208.175
 7.213001570D+05-3.832615200D+03 1.113963285D+01-2.238062246D-03 6.547723430D-07
-7.611335900D-11 3.328361050D-15                2.502497403D+04-4.305129910D+01
NO2-            EA,Cons: TPIS 1989 v1 pt1 p334; pt2 p208.
 2 tpis89 N   1.00O   2.00E   1.00    0.00    0.00 0   46.0060886    -200035.591
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10177.009
-1.282069477D+04 6.990140090D+02-2.812597149D+00 2.412894459D-02-2.831606955D-05
 1.670509541D-08-3.983330600D-12               -2.809915674D+04 4.063538160D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10177.009
 1.325705145D+05-1.557030905D+03 8.126720750D+00-2.728621269D-04-4.707555570D-08
 2.826730740D-11-2.353986343D-15               -1.715796019D+04-2.228309042D+01
NO2CL           TPIS 1989 v1 pt1 p391. NASA RP1271 1992 METHOD NRRAO1.
 2 g 4/99 N   1.00O   2.00CL  1.00    0.00    0.00 0   81.4582400      12500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12204.839
 8.508370340D+03-1.805383762D+02 3.785388560D+00 1.414934934D-02-1.423946765D-05
 7.028226180D-09-1.374688214D-12                9.156246470D+02 6.958899670D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12204.839
-1.086773327D+05-1.452231167D+03 1.105656962D+01-4.000099280D-04 9.101543040D-08
-1.036656913D-11 4.781664810D-16                6.294267320D+03-3.521240160D+01
NO2F            TPIS 1989 v1 pt1 p349. NASA RP1271 1992 METHOD NRRAO1.
 2 g 4/99 N   1.00O   2.00F   1.00    0.00    0.00 0   65.0039432    -109000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11346.581
 5.667856950D+04-6.538251950D+02 4.472771520D+00 1.368870672D-02-1.460533236D-05
 7.779227940D-09-1.689355106D-12               -1.102179443D+04 3.292083540D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11346.581
-1.008577842D+05-1.704722752D+03 1.122954945D+01-4.685215970D-04 1.047692566D-07
-1.189150595D-11 5.470307120D-16               -6.891719180D+03-3.849788400D+01
 NO3            JANAF 12/64. JPCRD v14 sup1 1985 p1537.
 2 j12/64 N   1.00O   3.00    0.00    0.00    0.00 0   62.0049400      71128.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10958.914
 3.405398410D+04 2.266670652D+02-3.793081630D+00 4.170732700D-02-5.709913270D-05
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 3.834158110D-08-1.021969284D-11 0.000000000D+00 7.088112200D+03 4.273091810D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10958.914
-3.943872710D+05-8.244263530D+02 1.061325843D+01-2.448749816D-04 5.406060320D-08
-6.195466750D-12 2.870000149D-16 0.000000000D+00 8.982011730D+03-3.444666500D+01
NO3-            Hf0,Cons: TPIS 1989 v1 pt1 p335; pt2 p209.
 2 tpis89 N   1.00O   3.00E   1.00    0.00    0.00 0   62.0054886    -310779.531
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10773.105
 9.204813610D+04-3.911171150D+02-2.354356764D-01 2.836042108D-02-3.461324080D-05
 2.081787460D-08-5.021601270D-12                -3.576411500D+04 2.299942405D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10773.105
-3.110005758D+05-1.369087552D+03 1.101342913D+01-4.036878820D-04 8.902086470D-08
-1.019733480D-11 4.723330790D-16                -3.364321090D+04-3.878432560D+01
NO3F            TPIS 1989 v1 pt1 p384; pt2 p245.
 2 tpis89 N   1.00O   3.00F   1.00    0.00    0.00 0   81.0033432      15000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14444.156
 6.472894860D+04-8.213214850D+02 6.194955440D+00 1.805430310D-02-1.996684730D-05
 1.124478570D-08-2.680010910D-12                4.206701470D+03-7.016322350D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14444.156
-3.412115070D+05-2.353823540D+03 1.628106250D+01-1.910371950D-03 4.690760060D-07
-5.685891240D-11 2.720829550D-15                9.760030990D+03-6.558090850D+01
N2              TPIS 1978 v1 pt2 p207.
 3 tpis78 N   2.00    0.00    0.00    0.00    0.00 0   28.0134800         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8670.104
 2.210371497D+04-3.818461820D+02 6.082738360D+00-8.530914410D-03 1.384646189D-05
-9.625793620D-09 2.519705809D-12                7.108460860D+02-1.076003316D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8670.104
 5.877124060D+05-2.239249073D+03 6.066949220D+00-6.139685500D-04 1.491806679D-07
-1.923105485D-11 1.061954386D-15                1.283210415D+04-1.586639599D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8670.104
 8.310139160D+08-6.420733540D+05 2.020264635D+02-3.065092046D-02 2.486903333D-06
-9.705954110D-11 1.437538881D-15                4.938707040D+06-1.672099736D+03
N2+             TPIS 1989 v1 pt1 p323;pt2 p200.
 3 tpis89 N   2.00E  -1.00    0.00    0.00    0.00 0   28.0129314    1509508.424
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.100
-3.474047470D+04 2.696222703D+02 3.164916370D+00-2.132239781D-03 6.730476400D-06
-5.637304970D-09 1.621756000D-12                1.790004424D+05 6.832978374D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.100
-2.845599002D+06 7.058893030D+03-2.884886385D+00 3.068677059D-03-4.361652310D-07
 2.102514545D-11 5.411996470D-16                1.340388483D+05 5.090897442D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.100
-3.712829770D+08 3.139287234D+05-9.603518050D+01 1.571193286D-02-1.175065525D-06
 4.144441230D-11-5.621893090D-16               -2.217361867D+06 8.436270989D+02
N2-
 2 J 9/77 N   2.00E   1.00    0.00    0.00    0.00 0   28.0140286     148617.443
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 3.882684800D+00-3.192444600D-03 8.522783800D-06
-7.340374600D-09 2.205681500D-12                1.679693500D+04 3.111805200D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 3.115675300D+00 1.458868800D-03-6.017314800D-07
 1.134842300D-10-7.965851800D-15                1.685905800D+04 6.389856000D+00
NCN             Hf0:TPIS,v2 pt1,1991. Cons:JPCRD v17 n2,1988 p269.
 2 g12/89 N   2.00C   1.00    0.00    0.00    0.00 0   40.0241800     500795.485
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10519.089
-7.446489560D+04 9.657342500D+02-1.464086630D+00 1.946557520D-02-2.048339610D-05
 1.082901100D-08-2.303124170D-12                5.421137850D+04 3.358166902D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10519.089
-1.487261010D+05-7.745490050D+02 7.995153010D+00-1.627330140D-04 2.892350020D-08
-3.017398580D-12 1.976991900D-16                6.192338540D+04-2.113086328D+01
cis-N2D2
 2 j 6/77 N   2.00D   2.00    0.00    0.00    0.00 0   32.0416840     207108.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10308.037
-2.743672520D+04 7.149722730D+02-2.223201100D+00 2.088709970D-02-1.821695130D-05
 8.843968540D-09-1.917982390D-12                2.062243310D+04 3.637074540D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10308.037
 8.798169130D+05-5.299395180D+03 1.355011670D+01-1.316659400D-03 2.755884740D-07
-3.036386440D-11 1.365370850D-15                5.407456060D+04-6.271245130D+01
N2F2            TPIS 1989 v1 pt1 p377; pt2 p237.
 2 tpis89 N   2.00F   2.00    0.00    0.00    0.00 0   66.0102864      62373.546
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12868.756
 1.543893150D+04-2.183635130D+02 3.890284250D+00 1.674017740D-02-2.056393090D-05
 1.258692110D-08-3.110498290D-12                7.052038700D+03 5.265868260D+00
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12868.756
-1.824883860D+05-9.534029960D+02 1.069795480D+01-2.759968700D-04 6.055439700D-08
-6.911215080D-12 3.192587230D-16                9.283466960D+03-3.246968590D+01
N2F4            TPIS 1989 v1 pt1 p380; pt2 p240.
 2 tpis89 N   2.00F   4.00    0.00    0.00    0.00 0  104.0070928     -22000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17811.571
 1.162896880D+05-1.538638600D+03 9.053934590D+00 2.862133560D-02-4.332305020D-05
 3.067647750D-08-8.455467880D-12                2.865169240D+03-2.476435680D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17811.571
-5.188073730D+05-6.703979060D+02 1.650130850D+01-2.007703560D-04 4.440719180D-08
-5.095697440D-12 2.362733050D-16               -5.280409680D+03-6.040665900D+01
N2H2            Hf0,Cons:TPIS 1989 v1 pt1 p356.Trans,cis,and 1,1 eql.
 2 g 5/99 N   2.00H   2.00    0.00    0.00    0.00 0   30.0293600     211858.756
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9996.961
-1.504005163D+05 2.346687716D+03-9.405430290D+00 3.284299800D-02-3.121920401D-05
 1.721283190D-08-4.014537220D-12                1.319384041D+04 7.832383030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9996.961
 6.217567870D+06-1.753952096D+04 2.022730509D+01-9.757297660D-04-4.208416740D-07
 1.117921171D-10-7.627102210D-15                1.374152574D+05-1.199559128D+02
NH2NO2          Aminyl Nitrite.Hf298,Cons:TPIS 1989v1 pt1 p370;pt2 p233.
 2 tpis89 N   2.00H   2.00O   2.00    0.00    0.00 0   62.0281600     -26000.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12163.853
-4.573035060D+04 1.201365987D+03-8.105984110D+00 5.402715200D-02-6.438074450D-05
 4.025097920D-08-1.025154190D-11 0.000000000D+00-9.615785160D+03 6.867353550D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12163.853
 1.654040575D+06-8.125220880D+03 2.021742772D+01-1.244291821D-03 2.122804183D-07
-1.948359653D-11 7.439351360D-16 0.000000000D+00 4.230822580D+04-1.016190160D+02
N2H4            Hf298,Cons:TPIS 1989 v1 pt1 p360;pt2 p225.
 2 g 4/99 N   2.00H   4.00    0.00    0.00    0.00 0   32.0452400      95180.000
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11449.304
-1.660756354D+05 3.035416736D+03-1.736889823D+01 7.159834020D-02-8.866799300D-05
 5.798970280D-08-1.530037218D-11 0.000000000D+00-3.731927230D+03 1.190002255D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11449.304
 3.293486700D+06-1.199850628D+04 2.104406814D+01-1.399381724D-03 1.933173351D-07
-1.318016127D-11 3.166400170D-16 0.000000000D+00 8.348433700D+04-1.155750987D+02
N2O             Hf298,Cons: TPIS 1989 v1 pt1 p337; pt2 p210.
 2 g 4/99 N   2.00O   1.00    0.00    0.00    0.00 0   44.0128800      81600.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9580.935
 4.288225970D+04-6.440118440D+02 6.034351430D+00 2.265394436D-04 3.472782850D-06
-3.627748640D-09 1.137969552D-12                1.179405506D+04-1.003128297D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9580.935
 3.438448040D+05-2.404557558D+03 9.125636220D+00-5.401667930D-04 1.315124031D-07
-1.414215100D-11 6.381066870D-16                2.198632638D+04-3.147804743D+01
N2O+            Nitrous oxide ion. IP & cons: JANAF p1555, 1970.
 2 j12/70 N   2.00O   1.00E  -1.00    0.00    0.00 0   44.0123314    1333000.000
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10623.407
-5.628613250D+04 6.701210350D+02 8.557988760D-02 1.524987320D-02-1.527923820D-05
 7.831271590D-09-1.647777390D-12                1.557322400D+05 2.563643140D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10623.407
-2.989955890D+04-1.179289530D+03 8.300023110D+00-2.886487230D-04 5.703172580D-08
-5.956495290D-12 2.834558070D-16                1.646063240D+05-2.287236830D+01
N2O3            Hf0,Cons: TPIS 1989 v1 pt1 p338; pt2 p211.
 2 g 4/99 N   2.00O   3.00    0.00    0.00    0.00 0   76.0116800      86630.595
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17120.855
-9.204444170D+04 9.295520150D+02 3.203664810D+00 1.356473078D-02-6.262966070D-06
-1.402915559D-09 1.431620930D-12                3.313622080D+03 1.844431111D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17120.855
 7.783881860D+05-4.483024660D+03 1.666668024D+01-2.062143878D-03 5.309541710D-07
-6.190451220D-11 2.692956658D-15                3.360912450D+04-6.739212230D+01
N2O4            Hf0,Cons: TPIS 1989 v1 pt1 p342; pt2 p212.
 2 tpis89 N   2.00O   4.00    0.00    0.00    0.00 0   92.0110800      11110.919
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16741.231
-3.804751440D+04 5.612828890D+02-2.083648324D-01 3.887087820D-02-4.422412260D-05
 2.498812310D-08-5.679102380D-12               -3.310794730D+03 2.963924970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16741.231
-4.582843760D+05-1.604749805D+03 1.674102133D+01-5.091385080D-04 1.143634670D-07
-1.316288176D-11 5.976316620D-16                4.306900520D+03-6.569450250D+01
N2O5            Hf298,Cons: TPIS 1989 v1 pt1 p343; pt2 p213.
 2 g 4/99 N   2.00O   5.00    0.00    0.00    0.00 0  108.0104800      13300.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20797.425
 4.007828170D+04-8.769675120D+02 1.055932981D+01 1.394613859D-02-8.884346920D-06
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 8.500431150D-10 7.791550910D-13                 3.038962037D+03-2.386831749D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20797.425
-5.325578960D+04-3.109277389D+03 2.036088958D+01-9.959901140D-04 2.401398635D-07
-3.057161911D-11 1.495915511D-15                 1.336957281D+04-8.298623230D+01
N3              Hf298,Cons: TPIS 1989 v1 pt1 p325;pt2 p202.
 2 tpis89 N   3.00    0.00    0.00    0.00    0.00 0   42.0202200     436000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9570.906
 3.337406790D+04-2.965683604D+02 3.314279150D+00 6.721685360D-03-4.181126390D-06
 8.618442360D-10 6.883352530D-14                 5.298840620D+04 5.312780770D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9570.906
 2.529264658D+05-2.362876591D+03 9.135267130D+00-6.212870850D-04 1.324094351D-07
-1.478989640D-11 6.721230470D-16                 6.412695390D+04-3.135825545D+01
N3H             Hf298,Cons: TPIS 1989 v1 pt1 p362;pt2 p226.
 2 g 4/99 N   3.00H   1.00    0.00    0.00    0.00 0   43.0281600     294000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10947.183
 3.242576060D+03 6.692664890D+01 1.766142217D+00 1.487411419D-02-1.539086440D-05
 9.172303550D-09-2.337205474D-12                 3.392069700D+04 1.513752475D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10947.183
 1.170469241D+06-5.102451990D+03 1.278288910D+01-8.409487160D-04 1.592142834D-07
-1.512289051D-11 6.102906630D-16                 6.428344470D+04-5.513118690D+01
Na              Hf:CODATA 1989 p27. Levels:JPCRD v10 n1 p153 1981
 3 g 8/97 NA  1.00    0.00    0.00    0.00    0.00 0   22.9897700     107500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.218382949D+04 4.244028180D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 9.525723380D+05-2.623807254D+03 5.162596620D+00-1.210218586D-03 2.306301844D-07
-1.249597843D-11 7.226771190D-16                 2.912963564D+04-1.519717061D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 1.592533392D+09-9.717836660D+05 2.238443963D+02-2.380930558D-02 1.352018117D-06
-3.936971110D-11 4.630689121D-16                 7.748677260D+06-1.939615505D+03
Na+             Spec:JPCRD v10 n1 1981 p153.
 3 g 4/97 NA  1.00E  -1.00    0.00    0.00    0.00 0   22.9892214     609542.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 7.256537070D+04 3.550845211D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 7.256537070D+04 3.550845211D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 3.401202990D+04-2.137774622D+01 2.505443851D+00-7.186631690D-07 5.188796390D-11
-1.944511626D-15 2.959355125D-20                 7.273413620D+04 3.503904191D+00
Na-             JPCRD v14 n3 1985 p731.
 3 g 4/97 NA  1.00E   1.00    0.00    0.00    0.00 0   22.9903186      48453.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.082199670D+03 3.550916790D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.082199670D+03 3.550916790D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000001D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.082199670D+03 3.550916790D+00
NaALF4
 2 J12/79 NA  1.00AL  1.00F   4.00    0.00    0.00 0  125.9649208   -1840979.855
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.305214500D+00 4.496803400D-02-7.432378700D-05
 5.808086100D-08-1.749955600D-11                -2.241498800D+05 6.371846002D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.427155300D+01 1.980019100D-03-8.815148400D-07
 1.732214800D-10-1.251291500D-14                -2.261234700D+05-4.127551799D+01
NaBO2
 2 J 6/71 NA  1.00B   1.00O   2.00    0.00    0.00 0   65.7995700    -648530.975
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.065474900D+00 1.345492600D-02-1.386669300D-05
 6.639504200D-09-1.072867100D-12                -7.970015700D+04 7.934816336D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.496525000D+00 2.630986200D-03-1.097913600D-06
 2.049399800D-10-1.419314600D-14                -8.057859100D+04-9.446301764D+00
NaBr
 2 J 9/64 NA  1.00BR  1.00    0.00    0.00    0.00 0  102.8937700    -143931.769
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   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.901089000D+00 2.502540100D-03-3.885108800D-06
 2.831849700D-09-7.722052800D-13              -1.855616100D+04 6.188793259D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.443313500D+00 1.578365700D-04-2.798961900D-08
 5.384903800D-12-3.809405400D-16              -1.865948900D+04 3.608582159D+00
NaCN
 2 J3/66  NA  1.00C   1.00N   1.00    0.00    0.00 0   49.0072100     94271.689
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.977255800D+00 5.322593700D-03-7.555244100D-06
 6.183979400D-09-2.007142700D-12               9.673149000D+03-3.882255844D-01
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.798977500D+00 1.682794600D-03-6.743792400D-07
 1.223450200D-10-8.296609100D-15               9.493344400D+03-4.344278713D+00
NaCL
 2 J12/64 NA  1.00CL  1.00    0.00    0.00    0.00 0   58.4424700   -181412.211
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.703228600D+00 3.199760800D-03-4.892450200D-06
 3.463921800D-09-9.135752100D-13              -2.302827600D+04 5.773479541D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.428293100D+00 1.562724100D-04-2.810838300D-08
 4.716357100D-12-2.883255700D-16              -2.317090000D+04 2.300974641D+00
NaF
 2 J12/68 NA  1.00F   1.00    0.00    0.00    0.00 0   41.9881732   -290453.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.748718330D+00 8.032432890D-03-1.515635230D-05
 1.335922460D-08-4.451652440D-12              -3.600020740D+04 8.681078191D+00
  1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.333767960D+00 2.568077770D-04-6.942326210D-08
 1.196796170D-11-7.493083930D-16              -3.627978720D+04 1.300463611D+00
NaF2-
 2 J12/68 NA  1.00F   2.00E   1.00    0.00    0.00 0   60.9871250   -669451.533
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.582688900D+00 1.060521100D-02-1.572050100D-05
 1.056729700D-08-2.641592000D-12              -8.223449700D+04 1.489207659D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.122319300D+00 4.188405500D-04-1.797229900D-07
 3.404122900D-11-2.375193500D-15              -8.275573000D+04-1.078667445D+01
NaH
 2 J 3/63 NA  1.00H   1.00    0.00    0.00    0.00 0   23.9977100    124260.983
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.120395000D+00 1.399621700D-03 2.214123400D-06
-3.995079500D-09 1.672617800D-12               1.394006500D+04 4.394561265D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.813057900D+00 8.564380000D-04-3.122681600D-07
 5.850247100D-11-4.051392400D-15               1.368306200D+04 4.841682120D-01
NaI
 2 G 6/72 NA  1.00I   1.00    0.00    0.00    0.00 0  149.8942400    -89120.307
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.040627500D+00 1.968711100D-03-3.054542400D-06
 2.255632300D-09-6.228683200D-13              -1.198804100D+04 6.459801070D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.458457000D+00 1.424127800D-04-1.692627500D-08
 3.896008700D-12-2.796631100D-16              -1.206684300D+04 4.475958770D+00
NaO
 2 J12/67 NA  1.00O   1.00    0.00    0.00    0.00 0   38.9891700     83684.358
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.442100700D+00 4.161724100D-03-6.311836800D-06
 4.447919900D-09-1.172048600D-12               8.901147700D+03 6.950325407D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.392415800D+00 2.132057400D-04-4.522059800D-08
 7.975182100D-12-5.173598900D-16               8.711899500D+03 2.388089707D+00
NaO-
 2 J12/67 NA  1.00O   1.00E   1.00    0.00    0.00 0   38.9897186   -121336.751
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.418685500D+00 4.211738200D-03-6.310464600D-06
 4.387351500D-09-1.137263900D-12              -1.575223400D+04 5.668556467D+00
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.386800800D+00 2.234467200D-04-4.821247200D-08
 8.572086200D-12-5.609433400D-16              -1.594626800D+04 1.013634867D+00
NaOH            JPCRD 1996 v25 n4 p1211.
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 2 g12/96 NA  1.00O   1.00H   1.00    0.00    0.00 0   39.9971100    -191000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11396.000
 3.442009070D+04-7.923184110D+02 8.997917230D+00-4.079812220D-03 3.065747028D-06
-5.118968820D-10-1.541071305D-13               -2.086952791D+04-2.510581332D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11396.000
 8.753815490D+05-2.342521554D+03 7.978476440D+00 1.016420889D-04-6.268456760D-08
 1.022705874D-11-5.713241340D-16               -9.509856480D+03-2.202315202D+01
NaOH+
 2 J12/71 NA  1.00O   1.00H   1.00E  -1.00    0.00 0   39.9965614     677830.540
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.350520400D+00 8.746501500D-03-1.464267300D-05
 1.135150100D-08-3.211002600D-12                7.994639900D+04 2.344840795D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.668854700D+00 1.225393000D-03-3.402956300D-07
 4.285326800D-11-1.959376000D-15                7.980651400D+04-3.424682605D+00
Na2
 2 J12/83 NA  2.00    0.00    0.00    0.00    0.00 0   45.9795400     142043.125
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.115682610D+00 2.529040400D-03-5.621686450D-06
 6.461716650D-09-2.751283100D-12                1.578246160D+04 3.686724460D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.962019000D+00-1.060495060D-03-4.392797690D-07
 3.051748100D-10-3.394888160D-14                1.499909270D+04-6.696136340D+00
Na2C2N2
 2 J 3/66 NA  2.00C   2.00N   2.00    0.00    0.00 0   98.0144200      -8776.984
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.036802900D+01 1.334854700D-02-1.991033400D-05
 1.615647500D-08-5.126455000D-12               -4.593752700D+03-2.054946120D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.257278600D+01 3.394731800D-03-1.361693400D-06
 2.472095900D-10-1.677325400D-14               -5.049102100D+03-3.107421620D+01
Na2CL2
 2 J12/64 NA  2.00CL  2.00    0.00    0.00    0.00 0  116.8849400    -566077.384
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.958395300D+00 8.396236000D-03-1.381711600D-05
 1.027766600D-08-2.864499400D-12               -7.072593900D+04-8.175324659D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.826200100D+00 1.918476300D-04-8.160874300D-08
 1.529818100D-11-1.055899400D-15               -7.107714900D+04-1.703610085D+01
Na2F2
 2 J12/68 NA  2.00F   2.00    0.00    0.00    0.00 0   83.9763464    -846432.824
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.821219100D+00 1.983639600D-02-3.061761400D-05
 2.133704000D-08-5.534431400D-12               -1.038900500D+05 2.366254840D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.433553000D+00 6.361158800D-04-2.762472000D-07
 5.291719000D-11-3.731035300D-15               -1.048011400D+05-1.975299185D+01
Na2O
 2 G10/74 NA  2.00O   1.00    0.00    0.00    0.00 0   61.9789400     -41417.546
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.778717700D+00 9.948771600D-03-1.481445600D-05
 1.000323900D-08-2.513787400D-12               -6.736020600D+03 1.799476287D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.147058200D+00 3.983309900D-04-1.740891100D-07
 3.356516200D-11-2.381080100D-15               -7.219126100D+03-9.634810513D+00
Na2O2H2          JPCRD 1996 v25 n4 p1211.
 2 g12/96 NA  2.00O   2.00H   2.00    0.00    0.00 0   79.9942200    -624000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19346.141
 1.089419856D+05-2.634831154D+03 2.306613766D+01-1.689324297D-02 1.673504355D-05
-7.821324260D-09 1.475080881D-12               -6.593133330D+04-9.803014682D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19346.141
 1.675692516D+06-4.704867320D+03 1.697338722D+01 1.961739745D-04-1.237016213D-07
 2.025394733D-11-1.133033808D-15               -4.856280750D+04-6.813442902D+01
Na2SO4
 2 J 6/78 NA  2.00S   1.00O   4.00    0.00    0.00 0  142.0431400   -1033641.566
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.072749800D+00 5.458204700D-02-7.854353300D-05
 5.510422100D-08-1.526667600D-11               -1.267695500D+05 1.666882634D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.520612800D+01 4.298426400D-03-1.900840900D-06
 3.718753000D-10-2.678045700D-14               -1.296735700D+05-4.765692166D+01
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Nb              Hf0:TPIS1982. Spec:NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 3/98 NB  1.00    0.00    0.00    0.00    0.00 0   92.9063800     723113.099
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8354.099
 7.889660670D+04-1.212813914D+03 1.034579819D+01-1.676630056D-02 1.979119979D-05
-1.218224409D-08 3.058098336D-12                9.165315140D+04-3.594742850D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8354.099
-1.096553196D+06 2.546650713D+03 2.236054882D+00-1.280029198D-03 8.464237990D-07
-1.486269508D-10 8.714309406D-15                6.879124550D+04 1.398169030D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8354.099
 1.818626365D+09-1.032414940D+06 2.308238005D+02-2.445004311D-02 1.395626888D-06
-4.087233010D-11 4.826490497D-16                8.359622560D+06-1.997797290D+03
Nb+             Spec:NSRDS-NBS 35 v2 1971. IP:NSRDS-NBS 34 1970.
 3 g 7/97 NB  1.00E  -1.00    0.00    0.00    0.00 0   92.9058314    1393604.675
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8589.075
 1.314447859D+05-2.000135035D+03 1.505024212D+01-2.996583942D-02 3.729868630D-05
-2.269869569D-08 5.449089902D-12                1.760054029D+05-6.224595520D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8589.075
-1.077639646D+06 2.159046421D+03 2.310604767D+00-5.363991760D-04 5.057915090D-07
-1.032401533D-10 6.629241280D-15                1.517945546D+05 1.210678502D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8589.075
 1.876113970D+07-2.202847919D+04 1.427004521D+01-2.295936786D-03 2.430819459D-07
-1.116131589D-11 1.836221996D-16                3.245415600D+05-8.494555710D+01
Nb-             JPCRD v14 n3 1985 p731.
 3 g 9/97 NB  1.00E   1.00    0.00    0.00    0.00 0   92.9069286     631054.008
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8653.808
-7.220924850D+04 5.259501250D+02 3.470468390D+00-4.950505530D-03 7.401859030D-06
-5.016302070D-09 1.314100719D-12                7.178828870D+04 5.155510070D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8653.808
 1.117458019D+05 1.340072834D+02 2.391474129D+00 4.524813430D-05-1.025345000D-08
 1.195577988D-12-5.606330450D-17                7.473996750D+04 9.675315610D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8653.808
-1.279446680D+05 1.664265071D+02 2.463334336D+00 4.161717840D-06-2.573750764D-10
 8.239892930D-15-1.069096936D-19                7.430433860D+04 9.186188470D+00
NbCL5           JANAF data.
 2 j12/74 NB  1.00CL  5.00    0.00    0.00    0.00 0  270.1698800    -703330.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26343.163
 7.348277970D+04-1.919172996D+03 2.290799567D+01-1.404352774D-02 1.638106985D-05
-1.018941843D-08 2.612266639D-12               -7.974118810D+04-8.439637920D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26343.163
-1.563816638D+05-4.450521280D+01 1.603544630D+01-1.489949737D-05 3.420777920D-09
-4.041124420D-13 1.917266128D-17               -8.962815120D+04-4.374583440D+01
NbO
 2 J12/73 NB  1.00O   1.00    0.00    0.00    0.00 0  108.9057800     198744.989
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.921448500D+00 3.132408200D-03-1.490036900D-06
-9.934526000D-10 7.998402000D-13                2.290788600D+04 1.123629370D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.881172900D+00 8.197812200D-04-4.253539000D-07
 1.026493600D-10-8.041980100D-15                2.263713200D+04 6.223641510D+00
NbOCL3          Barin 1989 w Wilhoit extrap. JPCRD v11 1982 sup2.
 2 bar 89 NB  1.00O   1.00CL  3.00    0.00    0.00 0  215.2638800    -752300.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20631.000
-1.108482359D+05 1.173066983D+02 1.165558433D+01 1.287422064D-03-1.659778281D-06
 1.102107826D-09-2.949903264D-13               -9.504023920D+04-2.386450719D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20631.000
-1.515551427D+05 5.305545230D+01 1.228915282D+01-1.527366571D-04 6.778576440D-08
-9.365170650D-12 4.670036930D-16               -9.490768120D+04-2.745264461D+01
NbO2
 2 J12/73 NB  1.00O   2.00    0.00    0.00    0.00 0  124.9051800    -200000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.576726810D+00 6.358956280D-03-5.964422090D-07
-6.342289560D-09 3.708328210D-12               -2.538731850D+04 1.062570080D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.051479480D+00 9.751537070D-04-3.826971080D-07
 6.541504200D-11-4.071590790D-15               -2.610086450D+04-2.400156630D+00
Ne              Ref-Elm. Moore: NSRDS-NBS 35 1971; NSRDS-NBS 34 1970.
 3 g 5/97 NE  1.00    0.00    0.00    0.00    0.00 0   20.1797000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.453750000D+02 3.355322720D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
```

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 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02 3.355322720D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.238252746D+07 6.958579580D+03 1.016709287D+00 1.424664555D-04-4.803933930D-09
-1.170213183D-13 8.415153652D-18              -5.663933630D+04 1.648438697D+01
Ne+            Moore: NSRDS-NBS 35 1971; NSRDS-NBS 34 1970.
 3 g 3/97 NE  1.00E  -1.00    0.00    0.00    0.00 0   20.1791514    2086965.946
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6304.214
 7.281551480D+04-8.695697990D+02 6.108646970D+00-5.841356930D-03 5.041044170D-06
-2.293759207D-09 4.339065680D-13              2.545996890D+05-1.673449355D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6304.214
-1.112742634D+05 4.765697940D+02 2.196650532D+00 1.102593149D-04-2.287564420D-08
 2.510218176D-12-1.126646091D-16              2.472536944D+05 7.466140530D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6304.214
-5.615094570D+04 1.418958835D+02 2.475717326D+00 1.944374235D-06-6.322736570D-11
-1.314511166D-16 3.534859008D-20              2.494452387D+05 5.366877980D+00
Ni             Hf0:Hultgren 1973. Levels:Physica Scripta v47 1993 p628.
 3 g 8/97 NI  1.00    0.00    0.00    0.00    0.00 0   58.6934000     430116.605
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6825.013
-3.235810550D+04 6.015264620D+02-1.079270657D+00 1.089505519D-02-1.369578748D-05
 8.317725790D-09-2.019206968D-12              4.813810810D+04 2.718829200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6825.013
-4.938262210D+05 1.092909991D+03 2.410485014D+00-1.599071827D-05-1.047414069D-08
 4.624795210D-12-4.448865218D-17              4.336072170D+04 9.677195600D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6825.013
 3.492669880D+08-1.654227575D+05 3.349869360D+01-3.527085900D-03 3.240060240D-07
-1.604177606D-11 2.935430214D-16              1.409017848D+06-2.672455567D+02
Ni+            Levels:JPCRD v14 sup2 1985.
 3 g 8/97 NI  1.00E  -1.00    0.00    0.00    0.00 0   58.6928514    1172594.573
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.773
-8.969386030D+04 1.173601500D+03-3.410620410D+00 1.390739137D-02-1.501714923D-05
 7.896337900D-09-1.648686761D-12              1.345589500D+05 4.031495160D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.773
-3.961999320D+06 1.017084853D+04-6.029331290D+00 2.770858029D-03-8.902077700D-08
-5.541000580D-11 5.235342833D-15              7.340395120D+04 7.137503100D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6205.773
 5.286662360D+07-3.719827100D+04 1.470794435D+01-1.489309517D-03 8.648712770D-08
-1.705443550D-12 5.049635419D-18              4.253204090D+05-9.590502160D+01
Ni-            JPCRD v14 n3 1985 p731.
 3 g 9/97 NI  1.00E   1.00    0.00    0.00    0.00 0   58.6939486     311764.357
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6207.157
-8.437624750D+04 1.135476552D+03-3.380615830D+00 1.423003786D-02-1.582586302D-05
 8.608840410D-09-1.875316029D-12              3.124307590D+04 3.998061300D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6207.157
-5.433424800D+05 1.182645330D+03 2.126441240D+00 3.730455940D-05 6.953608430D-09
-1.945719381D-12 1.271571579D-16              2.854759122D+04 1.043462235D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6207.157
 2.235741343D+06-7.539321100D+02 2.675777011D+00-2.056834268D-05 1.297167360D-09
-4.210909080D-14 5.520885950D-19              4.359114370D+04 5.724516640D+00
NiCL
 2 J 9/77 NI  1.00CL  1.00    0.00    0.00    0.00 0   94.1461000     182008.903
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.489775700D+00 3.183793000D-03-1.914891200D-06
-3.573631700D-10 4.607476800D-13              2.072593500D+04 9.549744360D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.583651400D+00-1.432957800D-03 8.520772300D-07
-1.488639300D-10 8.155162400D-15              2.005650500D+04-1.637321440D+00
NiCL2
 2 J 9/77 NI  1.00CL  2.00    0.00    0.00    0.00 0  129.5988000     -73932.233
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.560617700D+00 1.361371300D-02-2.366013300D-05
 1.961626400D-08-6.241729100D-12             -1.068357100D+04 6.236194160D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.387453000D+00 8.463759500D-04-4.314954200D-07
 9.359084600D-11-7.191513900D-15             -1.123585700D+04-7.188951040D+00
NiO
 2 G 2/84 NI  1.00O   1.00    0.00    0.00    0.00 0   74.6928000     314003.739
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.991968200D+00 3.330920800D-03-1.535247100D-06
-1.564083300D-09 1.212850100D-12              3.674209400D+04 9.821407360D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 4.104611400D+00 4.865916000D-04-1.878678400D-07
 3.553185500D-11-2.471516600D-15                3.644564500D+04 4.076796560D+00
NiS
 2 J12/76 NI  1.00S   1.00    0.00    0.00    0.00 0   90.7594000     357427.400
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.116810700D+00 4.017352800D-03-1.558391100D-06
-1.506353600D-09 9.368388100D-13                4.189685700D+04 1.146773510D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.916047200D+00 3.137745100D-04-2.970181300D-07
 8.017972400D-11-6.725741800D-15                4.132103200D+04 1.818987970D+00
O               D0(O2):CJP v32 1954 p110. Spec:NSRDS-NBS 3 sect 1976.
 3 g 5/97 O   1.00    0.00    0.00    0.00    0.00 0   15.9994000     249175.003
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6725.403
-7.953611300D+03 1.607177787D+02 1.966226438D+00 1.013670310D-03-1.110415423D-06
 6.517507500D-10-1.584779251D-13                2.840362437D+04 8.404241820D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6725.403
 2.619020262D+05-7.298722030D+02 3.317177270D+00-4.281334360D-04 1.036104594D-07
-9.438304330D-12 2.725038297D-16                3.392428060D+04-6.679585350D-01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6725.403
 1.779004264D+08-1.082328257D+05 2.810778365D+01-2.975232262D-03 1.854997534D-07
-5.796231540D-12 7.191720164D-17                8.890942630D+05-2.181728151D+02
O+              Spec:JPCRD v22 n5 1993.
 3 g 8/97 O   1.00E  -1.00    0.00    0.00    0.00 0   15.9988514    1568787.228
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.879352842D+05 4.393376760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.166513208D+05 6.665456150D+02 1.702064364D+00 4.714992810D-04-1.427131823D-07
 2.016595903D-11-9.107157762D-16                1.837191966D+05 1.005690382D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.143835383D+08 1.469518523D+05-3.680864540D+01 5.036164540D-03-3.087873854D-07
 9.186834870D-12-1.074163268D-16               -9.614208960D+05 3.426193080D+02
O-              Spec:TPIS 1989 v1 pt1 p93. EA:JPCRD v14 n3 1985 p731.
 3 g 1/97 O   1.00E   1.00    0.00    0.00    0.00 0   15.9999486     101846.192
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6570.792
-5.695857110D+03 1.099287334D+02 2.184719661D+00 5.326359800D-04-5.298878440D-07
 2.870216236D-10-6.524692740D-14                1.093287498D+04 6.729863860D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6570.792
 9.769363180D+03 7.159604780D+00 2.494961726D+00 1.968240938D-06-4.304174850D-10
 4.912083080D-14-2.271600083D-18                1.149554438D+04 4.837036440D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6570.792
 5.662391000D+02 7.572340320D+00 2.498352500D+00 1.862632395D-07-1.151227211D-11
 3.688814210D-16-4.793297600D-21                1.148426000D+04 4.813406590D+00
OD              TPIS 1989 v1 pt1 p135; pt2 p47.
 2 tpis89 O   1.00D   1.00    0.00    0.00    0.00 0   18.0135020      37221.508
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8999.108
 2.118691536D+04-2.785982360D+02 5.456210120D+00-6.148119830D-03 9.117670560D-06
-5.527812710D-09 1.239794711D-12 0.000000000D+00 4.711375030D+03-7.616618910D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8999.108
 7.832473160D+05-2.532992554D+03 5.952124650D+00-3.743595280D-04 4.959527620D-08
 3.454454730D-12-7.380626800D-16 0.000000000D+00 1.955142652D+04-1.568898441D+01
OD-             TPIS 1989 v1 pt1 p137; pt2 p48.
 2 tpis89 O   1.00D   1.00E   1.00    0.00    0.00 0   18.0140506    -145382.896
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8642.104
 5.606128320D+04-7.514156150D+02 7.544188470D+00-1.092083064D-02 1.503688938D-05
-9.351665840D-09 2.246466046D-12 0.000000000D+00-1.489548282D+04-2.106498377D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8642.104
 3.029467029D+05-1.079684654D+03 4.211417380D+00 6.260830070D-04-2.411665054D-07
 4.248425540D-11-2.387099102D-15 0.000000000D+00-1.162776255D+04-4.724898790D+00
OH              TPIS 1978 pt1 p110; pt2 p37.
 3 tpis78 O   1.00H   1.00    0.00    0.00    0.00 0   17.0073400      39344.106
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8813.106
-1.998858990D+03 9.300136160D+01 3.050854229D+00 1.529529288D-03-3.157890998D-06
 3.315446180D-09-1.138762683D-12 0.000000000D+00 3.239683480D+03 4.674110790D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8813.106
 1.017393379D+06-2.509957276D+03 5.116547860D+00 1.305299930D-04-8.284322260D-08
 2.006475941D-11-1.556993656D-15 0.000000000D+00 2.044487130D+04-1.101282337D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8813.106
 2.847234193D+08-1.859532612D+05 5.008240900D+01-5.142374980D-03 2.875536589D-07
-8.228817960D-12 9.567229020D-17 0.000000000D+00 1.468642377D+06-4.023555580D+02
OH+             Props:TPIS 1978 v1 pt2 p39.IP:TPIS 1989 v1 pt1 p117.
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 3 g 6/99 O   1.00H   1.00E  -1.00    0.00    0.00 0   17.0067914    1290331.503
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8603.103
 6.031630860D+04-7.573520300D+02 7.307752930D+00-9.506881670D-03 1.202555795D-05
-6.829026100D-09 1.501588659D-12 0.000000000D+00 1.578579989D+05-1.950106996D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8603.103
 5.040729100D+05-1.380052958D+03 4.125462200D+00 8.331948840D-04-3.442856290D-07
 6.792853950D-11-4.363872130D-15 0.000000000D+00 1.633157066D+05-3.997058490D+00
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8603.103
 1.158286700D+09-6.841280390D+05 1.576194558D+02-1.618421339D-02 8.846128780D-07
-2.475038507D-11 2.807730875D-16 0.000000000D+00 5.615528970D+06-1.351879042D+03
OH-             TPIS 1989 v1 pt1 p118; pt2 p32.
 2 tpis89 O   1.00H   1.00E   1.00    0.00    0.00 0   17.0078886    -143190.296
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8606.104
 2.910880827D+04-3.216904940D+02 4.851029050D+00-2.579035357D-03 2.004980024D-06
-7.956852960D-11-2.320495634D-13 0.000000000D+00-1.664039310D+04-7.121591300D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8606.104
 4.711331170D+05-8.572336690D+02 3.166181210D+00 1.233581296D-03-3.999244580D-07
 6.239081670D-11-3.354343220D-15 0.000000000D+00-1.200002214D+04 1.487736260D+00
O2              TPIS 1989 v1 pt1 p94; pt2 p9.
 3 tpis89 O   2.00    0.00    0.00    0.00    0.00 0   31.9988000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8680.104
-3.425563420D+04 4.847000970D+02 1.119010961D+00 4.293889240D-03-6.836300520D-07
-2.023372700D-09 1.039040018D-12               -3.391454870D+03 1.849699470D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8680.104
-1.037939022D+06 2.344830282D+03 1.819732036D+00 1.267847582D-03-2.188067988D-07
 2.053719572D-11-8.193467050D-16               -1.689010929D+04 1.738716506D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8680.104
 4.975294300D+08-2.866106874D+05 6.690352250D+01-6.169959020D-03 3.016396027D-07
-7.421416600D-12 7.278175770D-17               2.293554027D+06-5.530621610D+02
O2+             TPIS 1989 v1 pt1 p98; pt2 p11.
 3 tpis89 O   2.00E  -1.00    0.00    0.00    0.00 0   31.9982514    1171828.436
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9311.112
-8.607205450D+04 1.051875934D+03-5.432380470D-01 6.571166540D-03-3.274263750D-06
 5.940645340D-11 3.238784790D-13 0.000000000D+00 1.345544668D+05 2.902709750D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9311.112
 7.384654880D+04-8.459559540D+02 4.985164160D+00-1.611010890D-04 6.427083990D-08
-1.504939874D-11 1.578465409D-15 0.000000000D+00 1.446321044D+05-5.811230650D+00
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9311.112
-1.562125524D+09 1.161406778D+06-3.302504720D+02 4.710937520D-02-3.354461380D-06
 1.167968599D-10-1.589754791D-15 0.000000000D+00-8.857866270D+06 2.852035602D+03
O2-             Cons and Hf0: TPIS,v1 pt1 p100,1989.
 2 g 4/89 O   2.00E   1.00    0.00    0.00    0.00 0   31.9993486     -48027.921
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9349.611
 1.883944500D+04 1.149460260D+02 1.518926440D+00 8.015969400D-03-9.850349350D-06
 6.044019140D-09-1.486383640D-12               -7.101494390D+03 1.501182820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9349.611
-5.658355140D+04-2.366939790D+02 4.675739150D+00-2.192165820D-05 1.710076070D-08
-1.755629710D-12 8.237103690D-17               -5.960741020D+03-2.436205170D+00
O3              TPIS 1989 pt1 p101; pt2 p15.
 2 tpis89 O   3.00    0.00    0.00    0.00    0.00 0   47.9982000     141800.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10366.417
-1.276059932D+04 5.890077570D+02-2.543736048D+00 2.689273318D-02-3.526984570D-05
 2.311907537D-08-6.044181970D-12 0.000000000D+00 1.348768455D+04 3.850042910D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10366.417
-2.755126224D+07 7.152820680D+04-5.735735000D+01 2.067310388D-02 2.072539251D-07
-8.529354440D-10 8.327476650D-14 0.000000000D+00-4.532162040D+05 4.692492940D+02
P               Hf:CODATA 1989. Levels:JPCRD v14 n3 1985 p751.
 3 g 5/97 P   1.00    0.00    0.00    0.00    0.00 0   30.9737610     316500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.040866570D+01-7.639418650D-01 2.504563992D+00-1.381689958D-05 2.245585515D-08
-1.866399889D-11 6.227063395D-15               3.732421910D+04 5.359303481D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.261794642D+06-4.559838190D+03 8.918079310D+00-4.381401460D-03 1.454286224D-06
-2.030782763D-10 1.021022887D-14               6.541723960D+04-3.915974795D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.215392545D+07-4.566911180D+04 2.837245428D+01-4.483244040D-03 3.579413080D-07
-1.255311557D-11 1.590290483D-16               3.370905760D+05-2.056960928D+02
P+              Levels:JPCRD v14 n3 1985 p751.
 3 g 4/97 P   1.00E  -1.00    0.00    0.00    0.00 0   30.9732124    1336453.460
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8141.860
-7.316908110D+04 9.627979140D+02-3.693938050D-01 4.766778340D-03-4.574768580D-06
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 2.371262331D-09-5.131314900D-13                1.549406849D+05 2.376640762D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8141.860
-5.594249360D+05 1.722576545D+03 8.430381090D-01 6.287368940D-04-6.317195460D-08
-1.810842484D-12 4.318112570D-16                1.490493431D+05 1.845275207D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8141.860
 1.362531054D+07-8.717502380D+03 4.747426280D+00-1.620871933D-04-3.935548100D-10
 4.845613020D-13-7.448402970D-18                2.284649718D+05-1.346454894D+01
P-              JPCRD v14 n3 1985 p731.
 3 g 4/97 P   1.00E   1.00    0.00    0.00    0.00 0   30.9743096     238826.765
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6747.865
-1.008949093D+04 1.826468403D+02 1.962456304D+00 9.197377540D-04-9.214998630D-07
 5.012872360D-10-1.142677121D-13                2.703082432D+04 9.478137822D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6747.865
 1.543488016D+04 9.495009340D+00 2.493170861D+00 2.700167711D-06-5.949210390D-10
 6.823766290D-14-3.166959910D-18                2.797572693D+04 6.246793872D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6747.865
 1.724147889D+03 1.074832503D+01 2.497654940D+00 2.655333078D-07-1.642839012D-11
 5.268015350D-16-6.849362660D-21                2.795482976D+04 6.215849262D+00
PCL             TPIS 1989 v1 pt1 p431; pt2 p282.
 2 tpis89 P   1.00CL  1.00    0.00    0.00    0.00 0   66.4264610     134615.112
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9291.112
 3.488861700D+04-5.603119340D+02 6.264568480D+00-3.183364370D-03 3.495326840D-06
-2.091034291D-09 5.418758600D-13                1.774653764D+04-8.074578922D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9291.112
-3.471681510D+05 9.935557930D+02 3.399430270D+00 4.019711700D-04 8.295588390D-08
-3.090212484D-11 2.106384858D-15                8.433591150D+03 1.064901561D+01
PCL2            TPIS 1989 v1 pt1 p432; pt2 p283.
 2 tpis89 P   1.00CL  2.00    0.00    0.00    0.00 0  101.8791610     -54292.353
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12248.757
 5.190084500D+04-1.060904200D+03 1.058549940D+01-6.879917530D-03 7.620773180D-06
-4.530115470D-09 1.116671660D-12               -3.220331180D+03-2.753519242D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12248.757
-8.349833970D+04-2.625249470D+01 7.020361810D+00-8.388768680D-06 1.896784740D-09
-2.214879920D-13 1.041653550D-17               -8.742993680D+03-6.234032024D+00
PCL2-           TPIS 1989 v1 pt1 p433; pt2 p284.
 2 tpis89 P   1.00CL  2.00E   1.00    0.00    0.00 0  101.8797096    -356285.253
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12453.247
 4.934832770D+04-9.601590540D+02 9.884769700D+00-4.950202950D-03 4.946217870D-06
-2.678675201D-09 6.076723610D-13               -3.998072400D+04-2.413132578D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12453.247
-8.564986760D+04-3.185555940D+01 7.024494960D+00-1.002251172D-05 2.253747944D-09
-2.619657192D-13 1.227059658D-17               -4.503811430D+04-6.721531195D+00
PCL3            TPIS 1989 v1 pt1 p433; pt2 p285.
 2 tpis89 P   1.00CL  3.00    0.00    0.00    0.00 0  137.3318610    -289500.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15932.466
 7.717745470D+04-1.617650860D+03 1.536080470D+01-1.011077050D-02 1.103408340D-05
-6.476121020D-09 1.579151140D-12               -2.955893640D+04-5.244339671D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15932.466
-1.333076930D+05-4.145883210D+01 1.003186060D+01-1.301946160D-05 2.922916890D-09
-3.391869240D-13 1.586425530D-17               -3.800336680D+04-2.050738661D+01
PCL5            TPIS 1989 v1 pt1 p435; pt2 p286.
 2 tpis89 P   1.00CL  5.00    0.00    0.00    0.00 0  208.2372610    -376000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23305.466
 1.029070200D+05-2.515707460D+03 2.430114970D+01-1.564610690D-02 1.709873030D-05
-1.006011430D-08 2.460158790D-12               -3.722582370D+04-9.816336250D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23305.466
-2.255906890D+05-6.938542820D+01 1.605359630D+01-2.202156960D-05 4.971392290D-09
-5.799860050D-13 2.725970770D-17               -5.034234220D+04-4.872455950D+01
PF              TPIS 1989 v1 pt1 p425; pt2 p276.
 2 tpis89 P   1.00F   1.00    0.00    0.00    0.00 0   49.9721642     -47944.793
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8891.107
 2.227866728D+04-1.727508706D+02 3.085366934D+00 5.489718230D-03-8.247972540D-06
 5.868882910D-09-1.617252113D-12               -5.809279650D+03 7.709718850D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8891.107
-1.132572282D+06 3.200038550D+03 7.780502370D-01 1.969518902D-03-4.365818970D-07
 5.243648570D-11-2.618755712D-15               -2.766773009D+04 2.759312302D+01
PF+
 2 J 6/77 P   1.00F   1.00E  -1.00    0.00    0.00 0   49.9716156     901540.873
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.940212200D+00-5.378458200D-04 3.935610600D-06
-4.672619400D-09 1.744583800D-12                1.072525970D+05 4.518503250D+00
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   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.081618400D+00 4.950691000D-04-2.031980800D-07
 3.923484700D-11-2.783033700D-15                1.071458470D+05 3.444416650D+00
PF-
 2 J 6/77 P   1.00F   1.00E   1.00    0.00    0.00 0   49.9727128    -164050.119
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.595137600D+00 3.031290900D-03-4.406291400D-06
 3.158347500D-09-8.920626700D-13                -2.090409440D+04 5.869906490D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.303769100D+00 2.639263000D-04-9.877430300D-08
 1.871182100D-11-1.211025200D-15                -2.105814440D+04 2.412291490D+00
PFCL            TPIS 1989 v1 pt1 p437; pt2 p288.
 2 tpis89 P   1.00F   1.00CL  1.00    0.00    0.00 0   85.4248642    -283184.119
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11630.381
 5.490188530D+04-8.658679480D+02 7.944467650D+00 9.503779100D-04-3.339090210D-06
 3.023977817D-09-9.450377540D-13                -3.132843217D+04-1.440427413D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11630.381
-1.282143211D+05-9.739043550D+01 7.072661660D+00-2.903614134D-05 6.408504490D-09
-7.338993770D-13 3.396723170D-17                -3.600649260D+04-7.626498303D+00
PFCL-           TPIS 1989 v1 pt1 p438; pt2 p289.
 2 tpis89 P   1.00F   1.00CL  1.00E   1.00    0.00 0   85.4254128    -529269.107
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11742.793
 8.934336850D+04-1.266972513D+03 9.912194530D+00-3.877928300D-03 3.036692411D-06
-1.296559380D-09 2.324226580D-13                -5.894505710D+04-2.617050987D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11742.793
-1.231565150D+05-9.765861110D+01 7.074029570D+00-2.997070692D-05 6.685280620D-09
-7.722262200D-13 3.599382300D-17                -6.558817220D+04-8.208883327D+00
PFCL2           TPIS 1989 v1 pt1 p440; pt2 p292.
 2 tpis89 P   1.00F   1.00CL  2.00    0.00    0.00 0  120.8775642    -511925.340
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14867.760
 8.266560560D+04-1.512138928D+03 1.303404207D+01-2.903247162D-03 7.836652970D-07
 6.458340660D-10-3.737641820D-13                -5.644237870D+04-4.100906413D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14867.760
-1.864589813D+05-1.148004379D+02 1.008599754D+01-3.447456520D-05 7.627972010D-09
-8.753097430D-13 4.057788350D-17                -6.450472190D+04-2.174055308D+01
PFCL-           TPIS 1989 v1 pt1 p438; pt2 p289.
 2 tpis89 P   1.00F   1.00CL  1.00E   1.00    0.00 0   85.4254128    -529269.107
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11742.793
 8.934336850D+04-1.266972513D+03 9.912194530D+00-3.877928300D-03 3.036692411D-06
-1.296559380D-09 2.324226580D-13                -5.894505710D+04-2.617050987D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11742.793
-1.231565150D+05-9.765861110D+01 7.074029570D+00-2.997070692D-05 6.685280620D-09
-7.722262200D-13 3.599382300D-17                -6.558817220D+04-8.208883327D+00
PFCL4           TPIS 1989 v1 pt1 p442; pt2 p295.
 2 tpis89 P   1.00F   1.00CL  4.00    0.00    0.00 0  191.7829642    -635016.440
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21733.860
 1.412071573D+05-2.882471080D+03 2.387345233D+01-1.239510207D-02 1.141290085D-05
-5.705483820D-09 1.195229703D-12                -6.613478650D+04-9.859694489D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21733.860
-2.954375880D+05-1.325154294D+02 1.610005380D+01-4.035359170D-05 8.971130740D-09
-1.033288810D-12 4.804468350D-17                -8.135719400D+04-5.062404859D+01
PF2             TPIS 1989 v1 pt1 p426; pt2 p277.
 2 tpis89 P   1.00F   2.00    0.00    0.00    0.00 0   68.9705674    -513103.659
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11081.447
 5.524765720D+04-6.280517800D+02 5.137437920D+00 9.120673350D-03-1.468773760D-05
 1.081268450D-08-3.064944490D-12                -5.977541470D+04-1.689589472D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11081.447
-1.708467120D+05-1.692051540D+02 7.125491600D+00-4.990852850D-05 1.097335230D-08
-1.252870260D-12 5.784791140D-17                -6.338295840D+04-1.041715673D+01
PF2-            TPIS 1989 v1 pt1 p426; pt2 p278.
 2 tpis89 P   1.00F   2.00E   1.00    0.00    0.00 0   68.9711160    -709337.947
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11044.553
 1.404793057D+05-1.699945753D+03 1.036823971D+01-3.599587690D-03 1.961925800D-06
-3.829329870D-10-3.375549520D-14                -7.810434510D+04-3.217375182D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11044.553
-1.653976056D+05-1.640604822D+02 7.124091520D+00-5.015431400D-05 1.117302152D-08
-1.289308601D-12 6.004706670D-17                -8.700223320D+04-1.109074866D+01
PF2CL           TPIS 1989 v1 pt1 p439; pt2 p290.
 2 tpis89 P   1.00F   2.00CL  1.00    0.00    0.00 0  104.4232674    -735076.682
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13876.318
 8.397590160D+04-1.318075883D+03 1.017203515D+01 5.571231220D-03-1.100920478D-05
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 8.726383180D-09-2.567714099D-12              -8.381656170D+04-2.766013382D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13876.318
-2.409281185D+05-2.033484670D+02 1.015150769D+01-6.048367310D-05 1.333942001D-08
-1.526772528D-12 7.063339180D-17              -9.101110590D+04-2.417825980D+01
PF2CL3          TPIS 1989 v1 pt1 p442; pt2 p294.
 2 tpis89 P   1.00F   2.00CL  3.00    0.00    0.00 0  175.3286674    -878744.962
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20165.238
 1.842099543D+05-3.334402390D+03 2.388510873D+01-1.030943175D-02 7.356504220D-06
-2.498621785D-09 2.513997646D-13              -9.279549890D+04-1.027991579D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20165.238
-3.655272540D+05-2.029694160D+02 1.615238015D+01-6.118796570D-05 1.355610375D-08
-1.557129640D-12 7.224359970D-17              -1.104941533D+05-5.387308961D+01
PF3             TPIS 1989 v1 pt1 p427; pt2 p279.
 2 tpis89 P   1.00F   3.00    0.00    0.00    0.00 0   87.9689706    -957400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12936.493
 8.480635790D+04-1.102293400D+03 7.160469590D+00 1.438340980D-02-2.318220520D-05
 1.702299330D-08-4.811133520D-12              -1.111839790D+05-1.457514002D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12936.493
-2.957190080D+05-2.997175970D+02 1.022290380D+01-8.886121560D-05 1.957588710D-08
-2.238471970D-12 1.034767230D-16              -1.173746670D+05-2.777372472D+01
PF3CL2          TPIS 1989 v1 pt1 p441; pt2 p293.
 2 tpis89 P   1.00F   3.00CL  2.00    0.00    0.00 0  158.8743706   -1122022.916
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19047.184
 1.822497206D+05-3.089610245D+03 2.067710388D+01-1.168732391D-03-5.020540740D-06
 5.804573350D-09-1.965367906D-12              -1.228120667D+05-8.627977921D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19047.184
-4.223838050D+05-3.207965220D+02 1.624013000D+01-9.623655310D-05 2.129279712D-08
-2.443515401D-12 1.132904350D-16              -1.392642151D+05-5.531286311D+01
PF4CL           TPIS 1989 v1 pt1 p439; pt2 p291.
 2 tpis89 P   1.00F   4.00CL  1.00    0.00    0.00 0  142.4200738   -1364909.395
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18320.605
 1.804240323D+05-2.741096618D+03 1.680192838D+01 9.919315250D-03-2.025636171D-05
 1.617979147D-08-4.772611520D-12              -1.532382587D+05-6.679120281D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18320.605
-4.781140040D+05-4.264812830D+02 1.631812121D+01-1.271374903D-04 2.806715254D-08
-3.215166300D-12 1.488512118D-16              -1.680488362D+05-5.735845121D+01
PF5             TPIS 1989 v1 pt1 p429; pt2 p280.
 2 tpis89 P   1.00F   5.00    0.00    0.00    0.00 0  125.9657770   -1593300.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16537.609
 1.855725490D+05-2.436911810D+03 1.200979750D+01 2.339417780D-02-3.814030230D-05
 2.796183070D-08-7.870796730D-12              -1.814569910D+05-4.486301692D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16537.609
-5.669459520D+05-6.675695920D+02 1.649763280D+01-1.988560000D-04 4.390354510D-08
-5.029961580D-12 2.329023920D-16              -1.944335710D+05-6.261534162D+01
PH              TPIS 1989 v1 pt1 p420; pt2 p272.
 2 tpis89 P   1.00H   1.00    0.00    0.00    0.00 0   31.9817010    230752.104
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8648.104
 2.273633198D+04-3.972674060D+02 6.233697660D+00-9.181784600D-03 1.523328123D-05
-1.085888585D-08 2.929760547D-12               2.852768404D+04-1.095191197D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8648.104
 7.814730650D+05-3.038451204D+03 7.467481020D+00-1.837522255D-03 7.165947700D-07
-1.142128853D-10 6.175410560D-15               4.536260180D+04-2.467298140D+01
PH2             TPIS 1989 v1 pt1 p422; pt2 p273.
 2 tpis89 P   1.00H   2.00    0.00    0.00    0.00 0   32.9896410    119553.470
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9981.571
 1.555316010D+04-1.841675040D+02 4.895939500D+00-3.495564670D-03 1.053438600D-05
-8.377712680D-09 2.270810810D-12               1.409842920D+04-2.210803566D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9981.571
 1.127878160D+06-4.715220140D+03 1.021496410D+01-1.167563870D-03 2.150514790D-07
-1.624173970D-11 3.765999270D-16               4.183062920D+04-4.231609614D+01
PH2-            TPIS 1989 v1 pt1 p423; pt2 p274.
 2 tpis89 P   1.00H   2.00E   1.00    0.00    0.00 0   32.9901896     -9265.418
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9960.082
 6.950684490D+04-7.719162910D+02 7.383537620D+00-8.522947210D-03 1.474476507D-05
-9.847160810D-09 2.413107871D-12               1.582295850D+03-1.761306419D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9960.082
 1.382525815D+06-5.213400670D+03 1.021694832D+01-1.116316349D-03 2.215004171D-07
-2.338005187D-11 1.015580932D-15               2.990683733D+04-4.378711585D+01
PH3
 2 J 6/62 P   1.00H   3.00    0.00    0.00    0.00 0   33.9975810       5423.662
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 3.158193500D+00 2.494149200D-03 9.025525300D-06
-1.022790400D-08 3.283425000D-12              -4.612372520D+02 6.237224816D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.344879400D+00 6.577094100D-03-2.633675500D-06
 4.774466000D-10-3.235439000D-14              -8.161767520D+02 3.954796216D+00
PN              TPIS 1989 v1 pt1 p446; pt2 p299.
 2 tpis89 P   1.00N   1.00    0.00    0.00    0.00 0   44.9805010     171487.305
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8702.105
-5.103203840D+04 8.202926680D+02-1.392772765D+00 1.287989789D-02-1.401425371D-05
 7.775633460D-09-1.751539330D-12               1.573226520D+04 3.251070766D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8702.105
-2.495625593D+05 1.760438830D+02 4.144121960D+00 2.478018097D-04-5.674896300D-08
 4.263645120D-12 3.063920924D-16               1.770317267D+04 1.325518731D+00
PO              TPIS 1989 v1 pt1 p404; pt2 p258.
 2 tpis89 P   1.00O   1.00    0.00    0.00    0.00 0   46.9731610     -27857.687
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9390.113
-6.845754060D+04 1.141295708D+03-2.779556060D+00 1.678458047D-02-1.974879516D-05
 1.192602320D-08-2.927460912D-12              -9.847745040D+03 4.184328297D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9390.113
-3.366667440D+05 6.229355840D+02 3.565605460D+00 6.516620720D-04-2.061770841D-07
 3.184413230D-11-1.573691908D-15              -8.939790390D+03 6.954859188D+00
PO-             TPIS 1989 v1 pt1 p407; pt2 p259.
 2 tpis89 P   1.00O   1.00E   1.00    0.00    0.00 0   46.9737096    -140067.094
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8778.106
 5.434346320D+04-4.123623550D+02 3.746483880D+00 3.858636470D-03-5.963343040D-06
 4.278286360D-09-1.139722989D-12              -1.555810937D+04 3.404436468D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8778.106
-8.480294780D+02 3.470544870D+02 2.877890167D+00 1.622182445D-03-4.870190990D-07
 6.645752270D-11-3.395703760D-15              -1.987209540D+04 1.075444355D+01
POCL3           TPIS 1989 v1 pt1 p436; pt2 p287.
 2 tpis89 P   1.00O   1.00CL  3.00    0.00    0.00 0  153.3312610    -568400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17715.956
 4.793788160D+04-1.270388280D+03 1.367716460D+01 1.082672100D-03-1.736104060D-06
 8.460890640D-10-1.174661330D-13              -6.507571880D+04-4.314706821D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17715.956
-2.185937970D+05-5.080269680D+02 1.337784650D+01-1.510731050D-04 3.340986780D-08
-3.835329760D-12 1.779329880D-16              -7.009315090D+04-3.984747181D+01
POFCL2          TPIS 1989 v1 pt1 p444; pt2 p297.
 2 tpis89 P   1.00O   1.00F   1.00CL  2.00    0.00 0  136.8769642    -793889.312
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16454.188
 4.694061560D+04-1.069242600D+03 1.071284279D+01 9.491183300D-03-1.306412424D-05
 8.426906020D-09-2.140294969D-12              -9.274894990D+04-2.815078377D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16454.188
-2.707647503D+05-6.556502270D+02 1.348668421D+01-1.942765035D-04 4.291184490D-08
-4.921844800D-12 2.282079808D-16              -9.654392140D+04-4.164964152D+01
POF2CL          TPIS 1989 v1 pt1 p443; pt2 p296.
 2 tpis89 P   1.00O   1.00F   2.00CL  1.00    0.00 0  120.4226674   -1022607.040
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14896.360
 5.226438160D+04-9.691037700D+02 7.963635980D+00 1.755599796D-02-2.398693997D-05
 1.572376747D-08-4.079746000D-12              -1.202656893D+05-1.593967449D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14896.360
-3.347086590D+05-8.176104810D+02 1.360664320D+01-2.420426112D-04 5.343712720D-08
-6.126461350D-12 2.839570116D-16              -1.233401194D+05-4.496103811D+01
POF3            TPIS 1989 v1 pt1 p430; pt2 p281.
 2 tpis89 P   1.00O   1.00F   3.00    0.00    0.00 0  103.9683706   -1252000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14166.349
 2.966030710D+04-4.276705750D+02 3.669146100D+00 2.839493780D-02-3.768318000D-05
 2.449104540D-08-6.341972870D-12              -1.501124530D+05 5.160417996D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14166.349
-3.690602420D+05-1.005552540D+03 1.374529940D+01-2.971037110D-04 6.554526640D-08
-7.509987330D-12 3.478969910D-16              -1.499761730D+05-4.882214181D+01
PO2             TPIS 1989 v1 pt1 p408; pt2 p260.
 2 tpis89 P   1.00O   2.00    0.00    0.00    0.00 0   62.9725610    -281527.237
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10512.866
-6.372664990D+04 1.036736320D+03-2.877772160D+00 2.278127180D-02-2.567910930D-05
 1.465054290D-08-3.387981900D-12              -3.993542460D+04 4.425294967D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10512.866
 4.926013200D+05-2.605414730D+03 9.517554130D+00-1.180345060D-03 2.532839320D-07
-1.789860350D-11 1.799789900D-16              -2.028917940D+04-2.969705773D+01
PO2-            TPIS 1989 v1 pt1 p409; pt2 p261.
 2 tpis89 P   1.00O   2.00E   1.00    0.00    0.00 0   62.9731096    -597623.751
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    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 2.702440495D+04 2.939758551D+01 1.162695140D+00 1.599895857D-02-1.979226574D-05
 1.208845764D-08-2.956635813D-12                -7.285945280D+04 1.963113000D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 1.628679172D+06-5.989199860D+03 1.369318823D+01-3.623843720D-03 9.488198110D-07
-1.040308726D-10 4.019033480D-15                -3.685959570D+04-5.956796122D+01
PS              TPIS 1989 v1 pt1 p444; pt2 p298.
 2 tpis89 P   1.00S   1.00    0.00    0.00    0.00 0   63.0397610     150431.316
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9616.116
-7.689786800D+02-4.637824070D+01 4.104649170D+00 1.555262273D-03-2.315757288D-06
 1.661425178D-09-4.631238400D-13                1.707875808D+04 4.230675966D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9616.116
-2.702729081D+05 8.883548220D+02 3.169190120D+00 1.022480817D-03-3.803740480D-07
 7.019861880D-11-4.269122310D-15                1.121510462D+04 1.147336428D+01
P2              TPIS 1989 v1 pt1 p398; pt2 p255.
 2 tpis89 P   2.00    0.00    0.00    0.00    0.00 0   61.9475220     144000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8904.107
 3.053922510D+04-3.246177590D+02 4.022463810D+00 3.232094790D-03-5.511052450D-06
 4.195572930D-09-1.215032180D-12                1.796910870D+04 1.645350331D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8904.107
-7.806936490D+05 2.307910870D+03 1.411743130D+00 2.108237420D-03-7.360856620D-07
 1.259360120D-10-7.079752490D-15                1.329824740D+03 2.169741365D+01
P2O3            TPIS 1989 v1 pt1 p410; pt2 p262.
 2 tpis89 P   2.00O   3.00    0.00    0.00    0.00 0  109.9457220    -684645.274
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16094.881
-6.645753890D+04 7.580900550D+02 9.888436770D-01 2.859878730D-02-3.231142110D-05
 1.834525170D-08-4.212489300D-12                -8.820036740D+04 2.689914458D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16094.881
-2.175344110D+05-1.369902000D+03 1.401142960D+01-4.023856960D-04 8.868345780D-08
-1.015657280D-11 4.704356060D-16                -7.922757000D+04-4.739487232D+01
P2O4            TPIS 1989 v1 pt1 p411; pt2 p263.
 2 tpis89 P   2.00O   4.00    0.00    0.00    0.00 0  125.9451220    -933754.627
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17325.580
-4.376091260D+04 4.905102830D+02 9.643649370D-01 3.886073580D-02-4.675509220D-05
 2.812625630D-08-6.824406100D-12                -1.168997790D+05 2.379582767D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17325.580
-3.670114860D+05-1.638423730D+03 1.721188610D+01-4.826580150D-04 1.064461900D-07
-1.219610070D-11 5.650654580D-16                -1.090435930D+05-6.714276593D+01
P2O5            TPIS 1989 v1 pt1 p411; pt2 p264.
 2 tpis89 P   2.00O   5.00    0.00    0.00    0.00 0  141.9445220   -1124370.354
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22049.905
-2.999159220D+04-4.594506590D+01 6.987486830D+00 2.883302970D-02-3.104509530D-05
 1.643868680D-08-3.467942300D-12                -1.381901400D+05-3.400572711D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22049.905
-3.247080160D+05-2.016975080D+03 2.048699340D+01-5.910641150D-04 1.301993020D-07
-1.490682940D-11 6.903573410D-16                -1.306290160D+05-8.031642952D+01
P3              TPIS 1989 v1 pt1 p402; pt2 p256.
 2 tpis89 P   3.00    0.00    0.00    0.00    0.00 0   92.9212830     210000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12005.602
 4.693358950D+04-8.643589320D+02 8.734247530D+00 1.094534560D-05-1.998573320D-06
 2.096750510D-09-6.922889710D-13                2.774847340D+04-2.063587261D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12005.602
-1.253513060D+05-8.306734620D+01 7.561956770D+00-2.474403950D-05 5.457276930D-09
-6.244660570D-13 2.887724220D-17                2.308722280D+04-1.228310621D+01
P3O6            TPIS 1989 v1 pt1 p412; pt2 p265.
 2 tpis89 P   3.00O   6.00    0.00    0.00    0.00 0  188.9176830   -1575681.029
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23439.282
 2.014493813D+05-3.053488073D+03 1.602114098D+01 4.316889900D-02-6.376544260D-05
 4.422867920D-08-1.200020334D-11 0.000000000D+00-1.776503811D+05-6.556267890D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23439.282
-8.787968100D+05-1.651988071D+03 2.772258397D+01-4.859326700D-04 1.067867708D-07
-1.218015776D-11 5.614911960D-16 0.000000000D+00-1.909165548D+05-1.220665277D+02
P4              TPIS 1989 v1 pt1 p402; pt2 p257.
 2 tpis89 P   4.00    0.00    0.00    0.00    0.00 0  123.8950440      58900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14108.648
 1.205141850D+05-2.345711790D+03 1.773946550D+01-1.456314970D-02 1.587594090D-05
-9.314710310D-09 2.271491670D-12                1.608846480D+04-7.088590647D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14108.648
-1.858705860D+05-6.284546890D+01 1.004844880D+01-1.987668850D-05 4.482408440D-09
-5.226103670D-13 2.455791290D-17                3.848210920D+03-2.477297797D+01
P4O6            TPIS 1989 v1 pt1 p413; pt2 p266.
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 2 tpis89 P   4.00O   6.00    0.00    0.00    0.00 0  219.8914440   -1606000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24797.523
 3.760894750D+05-5.685832620D+03 2.914225450D+01 2.251532120D-02-4.510269630D-05
 3.588312690D-08-1.057572060D-11                -1.688562480D+05-1.451359851D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24797.523
-1.008997240D+06-8.872753990D+02 2.866064830D+01-2.636018940D-04 5.810940720D-08
-6.648086960D-12 3.074391930D-16                -1.997138900D+05-1.281853821D+02
P4O7            TPIS 1989 v1 pt1 p414; pt2 p267.
 2 tpis89 P   4.00O   7.00    0.00    0.00    0.00 0  235.8908440   -1984448.045
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26372.317
 3.218586960D+05-4.871444730D+03 2.454417068D+01 4.015509550D-02-6.524197150D-05
 4.756554180D-08-1.332975491D-11 0.000000000D+00-2.184517427D+05-1.181504792D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26372.317
-1.102947375D+06-1.511077128D+03 3.210979500D+01-4.371803760D-04 9.516639610D-08
-1.075204176D-11 4.911025680D-16 0.000000000D+00-2.429096540D+05-1.473140859D+02
P4O8            TPIS 1989 v1 pt1 p415; pt2 p268.
 2 tpis89 P   4.00O   8.00    0.00    0.00    0.00 0  251.8902440   -2302214.078
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        27946.336
 2.719326942D+05-4.118600390D+03 2.028714235D+01 5.685416990D-02-8.400739630D-05
 5.823389060D-08-1.578647160D-11 0.000000000D+00-2.604539703D+05-9.407162070D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        27946.336
-1.173177311D+06-2.200632995D+03 3.563010130D+01-6.489849740D-04 1.429623989D-07
-1.635821725D-11 7.571070760D-16 0.000000000D+00-2.783843144D+05-1.679636960D+02
P4O9            TPIS 1989 v1 pt1 p416; pt2 p269.
 2 tpis89 P   4.00O   9.00    0.00    0.00    0.00 0  267.8896440   -2613979.111
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        29521.355
 2.199916395D+05-3.336464940D+03 1.586413106D+01 7.402452330D-02-1.034835052D-04
 6.944438320D-08-1.840733450D-11 0.000000000D+00-3.018742692D+05-6.997967670D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        29521.355
-1.233696783D+06-2.917032808D+03 3.917757110D+01-8.736402980D-04 1.937914895D-07
-2.230510118D-11 1.037248818D-15 0.000000000D+00-3.129637516D+05-1.897176420D+02
P4O10           TPIS 1989 v1 pt1 p419; pt2 p271.
 2 tpis89 P   4.00O  10.00    0.00    0.00    0.00 0    283.88905   -2906223.447
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        31096.553
 1.670142268D+05-2.540243300D+03 1.136853403D+01 9.137812160D-02-1.231990626D-04
 8.081032230D-08-2.106787011D-11 0.000000000D+00-3.410151910D+05-4.643431340D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        31096.553
-1.337201132D+06-3.516382330D+03 4.260403310D+01-1.037406404D-03 2.287613089D-07
-2.620219946D-11 1.213529528D-15 0.000000000D+00-3.459515050D+05-2.115498906D+02
Pb              Hf:TPIS 1991. Spec:NSRDS-NBS 35 1971;NSRDS-NBS 34 1970.
 3 g 8/97 PB  1.00    0.00    0.00    0.00    0.00 0  207.2000000     195200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 1.213382285D+03-1.906116019D+01 2.619299546D+00-3.829519610D-04 6.688180450D-07
-6.061231080D-10 2.240022429D-13                2.282096238D+04 6.201369200D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-9.084313070D+06 2.672673180D+04-2.626244039D+01 1.358282305D-02-2.685523566D-06
 2.352432800D-10-7.324114532D-15               -1.481650666D+05 2.154011624D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 5.325474970D+08-2.751419152D+05 6.303031930D+01-6.813672740D-03 4.447489610D-07
-1.519361678D-11 2.043475665D-16                2.243651683D+06-5.225649900D+02
Pb+             Spec: NSRDS-NBS 35 v3 1971; NSRDS-NBS 34 1970.
 3 g10/97 PB  1.00E  -1.00    0.00    0.00    0.00 0  207.1994514     916996.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 9.486689040D+00-1.134955793D-01 2.500549799D+00-1.382464681D-06 1.906022991D-09
-1.368396828D-12 4.003528117D-16                1.095438901D+05 7.538855900D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 1.320690183D+06-4.096048010D+03 7.389101510D+00-2.807751909D-03 7.830991650D-07
-9.310600910D-11 4.016371727D-15                1.354347306D+05-2.722020908D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 4.101539500D+08-2.538072503D+05 6.239804790D+01-6.542962120D-03 3.507316530D-07
-8.114133770D-12 5.908352630D-17                2.122867468D+06-5.163550210D+02
Pb-             JPCRD v14 n3 1985 p731.
 3 g 9/97 PB  1.00E   1.00    0.00    0.00    0.00 0  207.2005486     153881.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.776226140D+04 8.235132100D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.776226140D+04 8.235132100D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
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 0.000000000D+00 0.000000000D+00                 1.776226140D+04 8.235132100D+00
PbBr            TPIS 1991 v2 pt1 p434; pt2 p360.
 2 g 5/99 PB  1.00BR  1.00    0.00    0.00    0.00 0  287.1040000      64816.771
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10141.571
-2.448102244D+03-4.561568460D+01 4.690915100D+00-3.772693540D-04 5.776249800D-07
-4.074088710D-10 1.195414717D-13                 6.661127570D+03 5.987351310D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10141.571
-1.525183022D+06 4.384560960D+03-1.457494375D-01 2.243065005D-03-4.459728560D-07
 4.650277540D-11-1.883880987D-15                 -2.168567966D+04 4.083717250D+01
PbBr2           TPIS 1991 v2 pt1 p437; pt2 p362.
 2 tpis91 PB  1.00BR  2.00    0.00    0.00    0.00 0  367.0080000    -103908.063
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15021.937
-6.172766360D+03-6.783207630D+01 7.273156140D+00-5.990596120D-04 7.358634610D-07
-4.743604810D-10 1.246922291D-13                 -1.427890796D+04-6.987992150D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15021.937
-1.320421479D+04-1.143074947D+00 7.000972540D+00-4.284471610D-07 1.018044861D-10
-1.234016791D-14 5.971337650D-19                 -1.462213750D+04 8.868582650D-01
PbBr3           TPIS 1991 v2 pt1 p438; pt2 p363.
 2 tpis91 PB  1.00BR  3.00    0.00    0.00    0.00 0  446.9120000    -104010.957
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19968.643
-1.164424250D+04-1.555151665D+02 1.062317321D+01-1.361947117D-03 1.668738791D-06
-1.073686019D-09 2.818250340D-13                 -1.478208304D+04-1.443758579D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19968.643
-2.787930766D+04-2.633265111D+00 1.000223199D+01-9.807761410D-07 2.326232632D-10
-2.815994460D-14 1.361283735D-18                 -1.556981182D+04-1.081765474D+01
PbBr4           TPIS 1991 v2 pt1 p439; pt2 p364.
 2 tpis91 PB  1.00BR  4.00    0.00    0.00    0.00 0  526.8160000    -182435.511
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25871.489
-1.176458199D+04-2.567166983D+02 1.402223292D+01-2.224117068D-03 2.716201994D-06
-1.743340164D-09 4.567359750D-13                 -2.462125551D+04-2.882020750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25871.489
-3.880216030D+04-4.382933770D+00 1.300369823D+01-1.620061335D-06 3.834130880D-10
-4.633967180D-14 2.237427066D-18                 -2.592327065D+04-2.287710636D+01
PbCL            TPIS 1991 v2 pt1 p427; pt2 p355.
 2 g 5/99 PB  1.00CL  1.00    0.00    0.00    0.00 0  242.6527000       8818.592
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9786.592
 1.788257950D+03-1.493961600D+02 5.078143430D+00-1.176338845D-03 1.485252781D-06
-9.412273680D-10 2.444834949D-13                 4.446822830D+02 2.295933029D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9786.592
-2.729079656D+05 8.181253650D+02 3.480545520D+00 6.872416640D-04-1.986796377D-07
 2.969187271D-11-1.311237083D-15                 -5.479868260D+03 1.287811647D+01
PbCL+
 2 J 6/73 PB  1.00CL  1.00E  -1.00    0.00    0.00 0  242.6521514      745609.101
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 3.960480800D+00 2.251138400D-03-3.555930200D-06
 2.613096500D-09-7.190128400D-13                 8.842137000D+04 7.587742850D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.459169700D+00 9.740730700D-05-4.882113400D-09
-2.547224600D-12 6.247087700D-16                 8.832584700D+04 5.213100650D+00
PbCL2           TPIS 1991 v2 pt1 p430; pt2 p357.
 2 tpis91 PB  1.00CL  2.00    0.00    0.00    0.00 0  278.1054000    -175547.471
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14002.529
 2.830580143D+03-3.134256659D+02 8.212827290D+00-2.585096173D-03 3.109456077D-06
-1.972978208D-09 5.123542480D-13                 -2.167569042D+04-9.219415480D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14002.529
-3.149192744D+04-5.565477580D+00 7.004599540D+00-1.986025455D-06 4.651719590D-10
-5.579137010D-14 2.678143570D-18                 -2.327439309D+04-2.140742521D+00
PbCL2+
 2 J 6/73 PB  1.00CL  2.00E  -1.00    0.00    0.00 0  278.1048514      816322.636
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 5.565387600D+00 5.746841700D-03-9.244504100D-06
 6.725688800D-09-1.831385800D-12                 9.633498500D+04 5.249054000D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 6.841883700D+00 1.979247300D-04-9.656282200D-08
 2.010644000D-11-1.324657900D-15                 9.609401800D+04-8.160434800D-01
PbCL3           TPIS 1991 v2 pt1 p432; pt2 p358.
 2 tpis91 PB  1.00CL  3.00    0.00    0.00    0.00 0  313.5581000    -177653.507
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18255.693
 8.623588970D+02-5.253152750D+02 1.203336337D+01-4.335184980D-03 5.215698350D-06
-3.310022380D-09 8.596970610D-13                 -2.180576379D+04-2.694207393D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18255.693
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-5.664412790D+04-9.329514790D+00 1.000771099D+01-3.329727570D-06 7.799330810D-10
-9.354606100D-14 4.490589700D-18              -2.448508643D+04-1.507491301D+01
PbCL4          TPIS 1991 v2 pt1 p433; pt2 p359.
 2 tpis91 PB  1.00CL  4.00    0.00    0.00    0.00 0  349.0108000    -327430.362
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23449.438
 1.739405796D+04-8.902139320D+02 1.637565058D+01-7.088992260D-03 8.432567340D-06
-5.305309390D-09 1.368671294D-12              -3.888215620D+04-4.850134300D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23449.438
-8.266679560D+04-1.639486405D+01 1.301336711D+01-5.716141400D-06 1.329368390D-09
-1.585922492D-13 7.581763610D-18              -4.343984220D+04-2.874559779D+01
PbF            TPIS 1991 v2 pt1 p419; pt2 p350.
 2 g 5/99 PB  1.00F   1.00    0.00    0.00    0.00 0  226.1984032     -98867.294
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9268.606
 2.774046901D+04-4.881827540D+02 6.094488380D+00-2.928815001D-03 3.249856590D-06
-1.919664382D-09 4.767333050D-13              -1.072846288D+04-5.396668060D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9268.606
-1.466759940D+06 4.097888130D+03 1.927628309D-01 2.031704917D-03-3.761107120D-07
 3.366846020D-11-9.970578180D-16              -3.966508440D+04 3.553061380D+01
PbF2           TPIS 1991 v2 pt1 p424; pt2 p352.
 2 tpis91 PB  1.00F   2.00    0.00    0.00    0.00 0  245.1968064    -443427.390
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12572.610
 5.920552280D+04-1.052529292D+03 1.028969284D+01-5.876346270D-03 6.102333130D-06
-3.424792640D-09 8.024025420D-13              -4.999050000D+04-2.525115478D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12572.610
-8.505899770D+04-3.074244334D+01 7.023346040D+00-9.455183590D-06 2.108489027D-09
-2.434212002D-13 1.133872429D-17              -5.552236770D+04-5.496073220D+00
PbF3           TPIS 1991 v2 pt1 p425; pt2 p353.
 2 tpis91 PB  1.00F   3.00    0.00    0.00    0.00 0  264.1952096    -489572.613
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15535.047
 8.553090870D+04-1.731036694D+03 1.556596150D+01-1.022225919D-02 1.089984998D-05
-6.269998820D-09 1.502616508D-12              -5.300335670D+04-5.335733480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15535.047
-1.459704258D+05-4.820396430D+01 1.003685845D+01-1.501095764D-05 3.362474990D-09
-3.896020710D-13 1.820152103D-17              -6.206869590D+04-2.006978661D+01
PbF4           TPIS 1991 v2 pt1 p426; pt2 p354.
 2 tpis91 PB  1.00F   4.00    0.00    0.00    0.00 0  283.1936128    -799925.173
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19626.227
 1.309963563D+05-2.307299499D+03 1.945201440D+01-1.024522729D-02 9.395874960D-06
-4.626894150D-09 9.450881430D-13              -8.804147460D+04-7.524645820D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19626.227
-2.132616322D+05-8.578621950D+01 1.306428551D+01-2.575563598D-05 5.693324590D-09
-6.526219550D-13 3.022341960D-17              -1.002908979D+05-3.590240280D+01
PbI            TPIS 1991 v2 pt1 p440; pt2 p365.
 2 g 5/99 PB  1.00I   1.00    0.00    0.00    0.00 0  334.1044700     108904.210
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10339.010
-2.400534472D+03-1.980857529D+01 4.587720980D+00-1.587561260D-04 3.027929920D-07
-2.255875370D-10 7.080151250D-14               1.183986539D+04 7.543778550D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10339.010
-1.778193642D+06 5.244009210D+03-1.298357449D+00 3.022968514D-03-7.259134480D-07
 9.473092130D-11-4.481385130D-15              -2.172399758D+04 4.982396560D+01
PbI2           TPIS 1991 v2 pt1 p443; pt2 p367.
 2 tpis91 PB  1.00I   2.00    0.00    0.00    0.00 0  461.0089400     -10252.630
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15247.370
-5.904986720D+03-4.833307030D+01 7.195438030D+00-4.298600090D-04 5.291412070D-07
-3.416402820D-10 8.991341920D-14              -3.107780155D+03 1.324773678D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15247.370
-1.088339477D+04-8.164418370D-01 7.000697300D+00-3.079876763D-07 7.331718140D-11
-8.899193880D-15 4.310712500D-19              -3.352096380D+03 2.458605463D+00
PbI3           TPIS 1991 v2 pt1 p444; pt2 p368.
 2 tpis91 PB  1.00I   3.00    0.00    0.00    0.00 0  587.9134100      21755.412
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21065.012
-1.014996331D+04-5.938078200D+01 1.024073798D+01-5.304694530D-04 6.538623030D-07
-4.225895720D-10 1.113029818D-13              -1.138482403D+02-8.975540500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21065.012
-1.624229573D+04-1.002945584D+00 1.000085839D+01-3.796679740D-07 9.046751720D-11
-1.098840054D-14 5.325388290D-19              -4.138258930D+02-7.579417110D+00
PbI4           TPIS 1991 v2 pt1 p445; pt2 p369.
 2 tpis91 PB  1.00I   4.00    0.00    0.00    0.00 0  714.8178800     -41226.459
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        27520.541
-1.217096972D+04-7.226317440D+01 1.329294204D+01-6.454660900D-04 7.955761850D-07
-5.141632830D-10 1.354188031D-13              -8.528148680D+03-2.010457498D+01
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        27520.541
-1.958477744D+04-1.223385179D+00 1.300104732D+01-4.633295690D-07 1.104213978D-10
-1.341397771D-14 6.501706110D-19                -8.893193200D+03-1.840570345D+01
PbO             TPIS 1991 v2 pt1 p413; pt2 p345.
 2 g 5/99 PB  1.00O   1.00    0.00    0.00    0.00 0  223.1994000      68136.508
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8961.508
 3.643734380D+04-4.514292740D+02 4.896702970D+00 9.635055510D-04-2.500640301D-06
 2.188591772D-09-6.790733670D-13                 9.404476750D+03-5.321320090D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8961.508
-9.752448710D+05 3.949629020D+03-2.170456860D+00 5.536889590D-03-2.317523802D-06
 4.615637180D-10-3.076209394D-14                -1.698711538D+04 4.792995170D+01
PbO2            TPIS 1991 v2 pt1 p416; pt2 p347.
 2 tpis91 PB  1.00O   2.00    0.00    0.00    0.00 0  239.1988000     136152.734
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12250.934
 7.071058290D+04-1.076757462D+03 9.401711730D+00-1.003861584D-03-1.233815617D-06
 1.858386979D-09-6.834621210D-13                 1.999645981D+04-2.503976748D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12250.934
-1.307796670D+05-7.314361450D+01 7.554083410D+00-2.143421561D-05 4.696464000D-09
-5.344972180D-13 2.460760535D-17                1.413386101D+04-1.252684909D+01
PbS             TPIS 1991 v2 pt1 p448; pt2 p371.
 2 g 5/99 PB  1.00S   1.00    0.00    0.00    0.00 0  239.2660000     127945.522
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9430.322
 1.680655959D+04-3.657319180D+02 5.802040870D+00-2.567349140D-03 2.988108386D-06
-1.825618236D-09 4.603105990D-13                1.588960681D+04-3.303767700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9430.322
 7.492339580D+05-6.822711710D+02 2.550167047D+00 3.403399710D-03-1.936152341D-06
 4.576797490D-10-3.348984370D-14                 2.024446514D+04 1.506278761D+01
PbS2            TPIS 1991 v2 pt1 p450; pt2 p372.
 2 tpis91 PB  1.00S   2.00    0.00    0.00    0.00 0  271.3320000     244049.005
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14021.205
 2.446375880D+04-6.654855460D+02 9.920201180D+00-4.924194380D-03 5.716906290D-06
-3.529488830D-09 8.971138350D-13                3.044310130D+04-2.295764446D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14021.205
-5.416700300D+04-1.343600342D+01 7.510700360D+00-4.497318630D-06 1.032444494D-09
-1.219580043D-13 5.785804650D-18                2.701229533D+04-8.714607040D+00
Pb2             TPIS 1991 v2 pt1 p404; pt2 p342.
 2 g 5/99 PB  2.00    0.00    0.00    0.00    0.00 0  414.4000000     305561.153
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10555.953
-8.433770730D+02-2.157962977D+01 4.625541690D+00-2.686221387D-04 6.731989960D-07
-5.931266200D-10 2.165117658D-13                3.549842980D+04 7.017507300D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10555.953
-1.424126706D+07 3.993447860D+04-3.642460700D+01 1.858314612D-02-3.486451220D-06
 2.716863770D-10-5.904850140D-15                -2.219095714D+05 3.064131252D+02
Rb              Hf:CODATA1989. NSRDS-NBS-35 v2 1971;NSRDS-NBS 34 1970.
 3 g 1/98 RB  1.00    0.00    0.00    0.00    0.00 0   85.4678000      80900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 1.352856616D+01-2.042232679D-01 2.501213823D+00-3.650619900D-06 5.884722670D-09
-4.842274720D-12 1.596211946D-15                8.985569210D+03 6.207005480D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-1.138274064D+06 3.804041940D+03-2.750899258D+00 3.891460700D-03-1.632296823D-06
 3.511893140D-10-2.521064422D-14                -1.466454849D+04 4.253442370D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 3.245192200D+08-3.493850870D+05 1.159097652D+02-1.492843123D-02 9.582385060D-07
-2.996233671D-11 3.657332046D-16                2.636178014D+06-9.586517230D+02
Rb+             Spec:NSRDS-NBS-35 v2 1971. IP:NSRDS-NBS 34 1970
 3 g 1/98 RB  1.00E  -1.00    0.00    0.00    0.00 0   85.4672514     490129.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.820327360D+04 5.520506920D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 5.820327360D+04 5.520506920D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 4.120352830D+07-2.920376515D+04 1.102096776D+01-1.311457972D-03 1.124752629D-07
-5.107819770D-12 9.622794537D-17                2.850166118D+05-6.672202250D+01
Rb-             JPCRD v14 n3 1985 p731.
 3 g 9/97 RB  1.00E   1.00    0.00    0.00    0.00 0   85.4683486      27818.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.600405796D+03 5.520526170D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
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 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.600405796D+03 5.520526170D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.600405796D+03 5.520526170D+00
RbOH            JPCRD v26 n4 1997 p1031.
 2 g 9/97 RB  1.00O   1.00H   1.00    0.00    0.00 0  102.4751400    -238000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11761.202
 1.213832721D+04-5.441411590D+02 8.459814640D+00-3.561526560D-03 2.992872390D-06
-7.280267400D-10-4.553847180D-14                -2.787262486D+04-1.913421991D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11761.202
 8.958583130D+05-2.332339000D+03 7.971192480D+00 1.044439355D-04-6.328257750D-08
 1.029358824D-11-5.743277790D-16                -1.515568947D+04-1.950051629D+01
Rb2O2H2         JPCRD v26 n4 1997 p1031.
 2 g 9/97 RB  2.00O   2.00H   2.00    0.00    0.00 0  204.9502800    -639000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23407.379
-4.577076530D+03-8.417631000D+02 1.704083828D+01-5.357882540D-03 3.951778770D-06
-2.051775094D-10-4.085416910D-13                -7.694982170D+04-5.435412780D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       23407.379
 1.792711652D+06-4.659406600D+03 1.693822422D+01 2.106246492D-04-1.269617470D-07
 2.063382927D-11-1.150861507D-15                -5.024117630D+04-6.027054920D+01
Rn              Ref-Elm. Spec:NSRDS-NBS 35 v3 1971 p228.
 3 g 5/97 RN  1.00    0.00    0.00    0.00    0.00 0  222.0176000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.389432090D-06-1.311675533D-07 2.500000001D+00-2.978593139D-12 4.337050730D-15
-3.182040220D-18 9.247787030D-22                -7.453749990D+02 6.952441980D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.730190029D+04-8.284672620D+01 2.598178483D+00-5.813729850D-05 1.819136527D-08
-2.866656182D-12 1.789322176D-16                -2.202809340D+02 6.255005710D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 9.180866680D+08-6.245854600D+05 1.724946531D+02-2.325758595D-02 1.636222413D-06
-5.369173150D-11 6.507189926D-16                4.883105900D+06-1.449516146D+03
Rn+             NSRDS-NBS 35 v3 1971 p230.
 3 g 1/97 RN  1.00E  -1.00    0.00    0.00    0.00 0  222.0170514    1043270.264
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-9.697148970D-02 1.106742047D-03 2.499994937D+00 1.189388239D-08-1.515895754D-11
 9.958934810D-15-2.640751817D-18                1.247304760D+05 8.338761700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.998285319D+04 5.930675660D+01 2.432476003D+00 3.716025920D-05-1.012057848D-08
 1.192256661D-12-3.184521980D-17                1.243528478D+05 8.821997790D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.408821471D+07 1.571151698D+04-1.411683762D+00 4.495267600D-04-2.324033616D-08
 5.830243350D-13-5.821682810D-18                9.187457500D+02 4.233613280D+01
S               Hf: CODATA 1989 p22. Levels:JPCRD v19 n4 1990 p821.
 3 g 5/97 S   1.00    0.00    0.00    0.00    0.00 0   32.0660000     277170.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6657.425
-3.174841820D+02-1.924704923D+02 4.686825930D+00-5.841365600D-03 7.538533520D-06
-4.863586040D-09 1.256976992D-12                3.323592180D+04-5.718477190D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6657.425
-4.854244790D+05 1.438830408D+03 1.258504116D+00 3.797990430D-04 1.630685864D-09
-9.547095850D-12 8.041466646D-16                2.334995270D+04 1.559559533D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6657.425
-1.302005414D+08 6.909362020D+04-1.176228025D+01 1.601540850D-03-1.050533340D-07
 4.341829020D-12-7.675621927D-17                -5.261485030D+05 1.322195719D+02
S+              Spec:JPCRD v19 n4 1990 p821.
 3 g 1/98 S   1.00E  -1.00    0.00    0.00    0.00 0   32.0654514    1282496.428
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 1.535026117D+05 5.436270120D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.346218684D+06-4.056871510D+03 7.153436550D+00-2.523562352D-03 6.429539610D-07
-6.431672160D-11 2.141387919D-15                1.792823835D+05-2.786930401D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.542254583D+08-1.023073546D+05 2.591796942D+01-2.111469141D-03 9.215571560D-08
-1.964168821D-12 2.096218597D-17                9.622418410D+05-2.017239489D+02
S-              JPCRD v14 n3 1985 p731.
 3 g 4/97 S   1.00E   1.00    0.00    0.00    0.00 0   32.0665486      70368.505
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6464.905
-2.596051473D+03-1.422398653D+02 4.007825670D+00-3.608855910D-03 4.236230000D-06
-2.520987604D-09 6.079479760D-13                8.197793070D+03-2.582330567D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6464.905
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 2.730311692D+03 1.414072078D+02 2.403340775D+00 3.693577530D-05-7.944080440D-09
 8.952208380D-13-4.099662820D-17                6.931195700D+03 6.575033680D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6464.905
-1.223682088D+05 1.203125842D+02 2.473942293D+00 2.935459895D-06-1.808577869D-10
 5.778854260D-15-7.490337240D-20                6.947841220D+03 6.070626550D+00
SCL
 2 J 6/78 S   1.00CL  1.00    0.00    0.00    0.00 0   67.5187000     156469.988
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.705588000D+00 5.271862300D-03-1.137182000D-05
 1.049782700D-08-3.531840800D-12                1.756115900D+04 6.279451230D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.594726000D+00-5.977178600D-05 4.522649500D-08
-9.371843500D-12 8.073572700D-16                1.745242600D+04 2.379851530D+00
SCL2
 2 J 6/78 S   1.00CL  2.00    0.00    0.00    0.00 0  102.9714000     -17572.262
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.596637100D+00 1.432719300D-02-2.519919700D-05
 2.057288200D-08-6.397690800D-12               -3.637583700D+03 1.006055570D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.627146200D+00 4.274701900D-04-1.881688100D-07
 3.576115500D-11-2.384940000D-15               -4.200021900D+03-4.232370250D+00
SCL2+
 2 J 6/78 S   1.00CL  2.00E  -1.00    0.00    0.00 0  102.9708514     901508.596
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.595872700D+00 1.429166500D-02-2.508499800D-05
 2.044689300D-08-6.350466900D-12                1.069028300D+05 1.075583370D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.580257000D+00 5.217640000D-04-2.507697900D-07
 5.098812400D-11-3.273029200D-15                1.063548600D+05-3.294938320D+00
SD
 2 J 6/77 S   1.00D   1.00    0.00    0.00    0.00 0   34.0801020     138494.852
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.728559700D+00-5.093988100D-03 9.913460500D-06
-7.329081300D-09 1.946160800D-12                1.539957900D+04-1.568479520D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.347198800D+00 1.212964600D-03-4.773013800D-07
 8.832366900D-11-6.074059100D-15                1.562714700D+04 4.877641980D+00
SF             TPIS 1989 v1 pt1 p302;pt2 p183.
 2 tpis89 S   1.00F   1.00    0.00    0.00    0.00 0   51.0644032      15445.561
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9470.114
 1.206456680D+04-2.910270690D+02 5.480101520D+00-1.975880100D-03 2.473685790D-06
-1.610904480D-09 4.310038110D-13                1.991337530D+03-4.544109340D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9470.114
 7.634562400D+05-2.423633900D+03 7.352194440D+00-1.598024070D-03 4.868510040D-07
-6.477994310D-11 2.980294230D-15                1.577458620D+04-1.902578770D+01
SF+
 2 J 6/76 S   1.00F   1.00E  -1.00    0.00    0.00 0   51.0638546     991925.691
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.666664800D+00 5.697549100D-03-7.605742200D-06
 4.911945500D-09-1.241451400D-12                1.183103300D+05 1.051501930D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.280724800D+00 1.036743300D-04 5.544166500D-08
-1.143329500D-11 5.584690600D-16                1.179219200D+05 2.459394670D+00
SF-            TPIS 1989 v1 pt1 p304;pt2 p184.
 2 tpis89 S   1.00F   1.00E   1.00    0.00    0.00 0   51.0649518    -231346.893
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8875.107
 5.019879280D+04-5.321549310D+02 4.904849010D+00 9.915307420D-04-2.270841545D-06
 1.844749756D-09-5.357057200D-13               -2.611388646D+04-3.637438690D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8875.107
 2.068923125D+05-1.324372811D+03 6.646211240D+00-1.641781588D-03 6.783883120D-07
-1.198331099D-10 7.121739540D-15               -2.150994816D+04-1.470236246D+01
SF2            TPIS 1989 v1 pt1 p305;pt2 p185.
 2 tpis89 S   1.00F   2.00    0.00    0.00    0.00 0   70.0628064    -293188.734
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11048.373
 6.870539970D+04-8.431961170D+02 6.269252870D+00 6.484788500D-03-1.145217410D-05
 8.770940010D-09-2.542796280D-12               -3.230002770D+04-8.798639690D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11048.373
-1.703355800D+05-1.494914990D+02 7.110700540D+00-4.395102480D-05 9.646734290D-09
-1.099553520D-12 5.068868010D-17               -3.704425480D+04-1.095083960D+01
SF2+
 2 J12/76 S   1.00F   2.00E  -1.00    0.00    0.00 0   70.0622578     702406.521
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   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.427149000D+00 1.551754600D-02-2.306025900D-05
 1.649961200D-08-4.624641800D-12              8.323955700D+04 1.412788660D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.120900000D+00 9.998481700D-04-4.399293200D-07
 8.436813700D-11-5.779537800D-15              8.244458500D+04-3.863075420D+00
SF2-
 2 J12/76 S   1.00F   2.00E   1.00    0.00    0.00 0   70.0633550    -398434.655
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.290050300D+00 1.553861200D-02-2.723660400D-05
 2.218279900D-08-6.886215600D-12             -4.939192500D+04 9.817477630D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.584712300D+00 4.788609000D-04-2.140544000D-07
 4.217570300D-11-3.052391000D-15             -5.000570500D+04-5.733347870D+00
SF3          TPIS 1989 v1 pt1 p306;pt2 p186.
 2 tpis89 S   1.00F   3.00    0.00    0.00    0.00 0   89.0612096    -504101.395
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13548.265
 1.284001040D+05-2.084858550D+03 1.423412520D+01-4.014749900D-03 9.147494470D-07
 1.110203240D-09-5.989852830D-13             -5.239523160D+04-5.187146950D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13548.265
-2.410940390D+05-1.419816390D+02 1.010598930D+01-4.235430220D-05 9.345203200D-09
-1.069728880D-12 4.948467450D-17             -6.358389310D+04-2.489621480D+01
SF3+
 2 J12/76 S   1.00F   3.00E  -1.00    0.00    0.00 0   89.0606610     393598.441
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.001850800D+00 2.975515500D-02-4.335679400D-05
 3.055496400D-08-8.463347900D-12              4.604418400D+04 1.944450080D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.138501600D+00 2.128891400D-03-9.483682200D-07
 1.860743600D-10-1.327172900D-14              4.448673000D+04-1.542124220D+01
SF3-         TPIS 1989 v1 pt1 p307;pt2 p187.
 2 tpis89 S   1.00F   3.00E   1.00    0.00    0.00 0   89.0617582    -790124.207
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13722.893
 1.546500675D+05-2.469768526D+03 1.657548496D+01-1.020137434D-02 9.368008460D-06
-4.725672600D-09 1.009661431D-12             -8.500157900D+04-6.532164790D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13722.893
-2.253860964D+05-1.308890242D+02 1.009972380D+01-4.052345530D-05 9.064565220D-09
-1.049320641D-12 4.899201260D-17             -9.800227200D+04-2.524366339D+01
SF4          TPIS 1989 v1 pt1 p307;pt2 p188.
 2 tpis89 S   1.00F   4.00    0.00    0.00    0.00 0  108.0596128    -760000.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15382.882
 1.636202310D+05-2.531348180D+03 1.559127440D+01 3.326026910D-03-1.054821030D-05
 9.390406770D-09-2.914506320D-12             -8.115544140D+04-6.131644230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15382.882
-3.776532920D+05-2.939333660D+02 1.321921800D+01-8.758767660D-05 1.933140660D-08
-2.214088030D-12 1.024954480D-16             -9.483064570D+04-4.243201400D+01
SF4+
 2 J12/76 S   1.00F   4.00E  -1.00    0.00    0.00 0  108.0590642     416056.406
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.961581300D+00 4.213209400D-02-6.915556500D-05
 5.372066600D-08-1.610589500D-11              4.809474000D+04 1.637990080D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.135194100D+01 1.887566200D-03-8.390406200D-07
 1.641493800D-10-1.173519500D-14              4.622476700D+04-2.857150820D+01
SF4-
 2 J12/76 S   1.00F   4.00E   1.00    0.00    0.00 0  108.0601614    -887483.605
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.079376200D+00 3.783950300D-02-6.690465700D-05
 5.482243400D-08-1.709284400D-11             -1.091464200D+05 5.641787750D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.200332600D+01 1.200771300D-03-5.739827400D-07
 1.229938500D-10-9.295273400D-15             -1.106030800D+05-3.165926510D+01
SF5          TPIS 1989 v1 pt1 p308;pt2 p189.
 2 tpis89 S   1.00F   5.00    0.00    0.00    0.00 0  127.0580160    -902663.287
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18811.479
 2.224220060D+05-4.044056330D+03 2.707234700D+01-1.744289000D-02 1.604376300D-05
-7.998661030D-09 1.668415620D-12             -9.220047650D+04-1.232447010D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18811.479
-3.893879250D+05-1.821765790D+02 1.613721270D+01-5.521382770D-05 1.224842670D-08
-1.407925090D-12 6.534069080D-17             -1.135697160D+05-5.577207700D+01
SF5+
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 2 J12/77 S   1.00F   5.00E  -1.00    0.00    0.00 0  127.0574674     172651.429
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.716486100D+00 6.894004600D-02-1.147105100D-04
 8.997786500D-08-2.716632600D-11                1.906114900D+04 2.944451330D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.368421600D+01 2.517702300D-03-1.085439300D-06
 2.253374500D-10-1.722391700D-14                1.600490800D+04-4.419972370D+01
SF5-            TPIS 1989 v1 pt1 p309;pt2 p190.
 2 tpis89 S   1.00F   5.00E   1.00    0.00    0.00 0  127.0585646   -1204622.287
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19049.913
 2.095031134D+05-3.930081140D+03 2.702127215D+01-1.792973203D-02 1.718122152D-05
-9.000560190D-09 1.988018147D-12               -1.291816581D+05-1.231672739D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19049.913
-3.733219200D+05-1.793729521D+02 1.613699748D+01-5.577539970D-05 1.249477046D-08
-1.448104799D-12 6.767462300D-17               -1.498554401D+05-5.631438210D+01
SF6             TPIS 1989 v1 pt1 p311;pt2 p191.
 2 tpis89 S   1.00F   6.00    0.00    0.00    0.00 0  146.0564192   -1219400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16940.067
 3.309447920D+05-4.737578830D+03 2.247683200D+01 1.047094080D-02-2.560828680D-05
 2.153842000D-08-6.516429390D-12               -1.255365740D+05-1.091729100D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16940.067
-7.306733740D+05-6.366991720D+02 1.947441780D+01-1.894251740D-04 4.178446940D-08
-4.783204710D-12 2.213099900D-16               -1.510610210D+05-8.147566140D+01
SF6-
 2 J 6/77 S   1.00F   6.00E   1.00    0.00    0.00 0  146.0569678   -1341907.911
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-3.260927200D+00 8.269536900D-02-1.329981200D-04
 1.017376800D-07-3.014638300D-11               -1.631086000D+05 3.542334420D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.542864600D+01 4.084531700D-03-1.816490300D-06
 3.566732800D-10-2.575000000D-14               -1.668988400D+05-5.439612180D+01
SH              TPIS 1989 v1 pt1 p296;pt2 p179.
 2 tpis89 S   1.00H   1.00    0.00    0.00    0.00 0   33.0739400     140412.109
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9098.109
 6.389434680D+03-3.747960920D+02 7.548145770D+00-1.288875477D-02 1.907786343D-05
-1.265033728D-08 3.235158690D-12                1.722177180D+04-1.760757308D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9098.109
 1.682631601D+06-5.177152210D+03 9.198168520D+00-2.323550224D-03 6.543914780D-07
-8.468470420D-11 3.864741550D-15                4.878489270D+04-3.770395740D+01
SH-             TPIS 1989 v1 pt1 p297;pt2 p180.
 2 tpis89 S   1.00H   1.00E   1.00    0.00    0.00 0   33.0744886     -88297.296
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8646.104
 3.878070760D+04-5.742590600D+02 6.898544460D+00-1.001352412D-02 1.486460572D-05
-9.750368900D-09 2.446909813D-12               -8.942641120D+03-1.615961954D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8646.104
 1.198715402D+06-3.894846820D+03 7.660422330D+00-1.355237590D-03 3.342370240D-07
-3.350722310D-11 9.055084780D-16                1.296752173D+04-2.818366081D+01
SN              TPIS 1989 v1 pt1 p392;pt2 p252.
 2 tpis89 S   1.00N   1.00    0.00    0.00    0.00 0   46.0727400     267388.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9393.113
-6.835412350D+04 1.147567483D+03-2.877802574D+00 1.724864320D-02-2.058999904D-05
 1.261369640D-08-3.139030141D-12                2.564143612D+04 4.224010350D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9393.113
-4.837284460D+05 1.058075590D+03 3.086198804D+00 9.111360780D-04-2.764061722D-07
 4.157370110D-11-2.128351755D-15                2.379345477D+04 1.033225525D+01
SO              TPIS 1989 v1 pt1 p286;pt2 p173.
 2 tpis89 S   1.00O   1.00    0.00    0.00    0.00 0   48.0654000       4760.306
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8798.106
-3.342757000D+04 6.403862500D+02-1.006641228D+00 1.381512705D-02-1.704486364D-05
 1.061294930D-08-2.645796205D-12               -3.371292190D+03 3.093865084D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8798.106
-1.443410557D+06 4.113874360D+03-5.383695780D-01 2.794153269D-03-6.633352260D-07
 7.838221190D-11-3.560509070D-15               -2.708838059D+04 3.615361450D+01
SO-             TPIS 1989 v1 pt1 p288;pt2 p174.
 2 tpis89 S   1.00O   1.00E   1.00    0.00    0.00 0   48.0659486    -105968.086
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9467.114
 8.420196970D+03-6.916586680D+01 3.837666610D+00 2.166482062D-03-2.811222562D-06
 1.793426453D-09-4.521795950D-13               -1.354162531D+04 4.316172810D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9467.114
 1.767156147D+05-6.633987360D+02 5.177279810D+00-2.853461125D-04 7.214421530D-08
-3.676469490D-12-2.910092894D-16               -9.984438010D+03-3.951425550D+00
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SOF2            TPIS 1989 v1 pt1 p312;pt2 p192.
 2 tpis89 S   1.00O   1.00F   2.00    0.00    0.00 0   86.0622064    -584952.313
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12624.845
 6.114286670D+04-9.080697340D+02 6.883385530D+00 1.192526880D-02-1.671107440D-05
 1.110800550D-08-2.911020370D-12                -6.742956040D+04-1.125325210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12624.845
-2.511409310D+05-6.072007890D+02 1.045019970D+01-1.794935780D-04 3.960089660D-08
-4.537371280D-12 2.101886470D-16                -7.072227500D+04-2.904140670D+01
SO2             TPIS 1989 v1 pt1 p288; pt2 p175.
 2 tpis89 S   1.00O   2.00    0.00    0.00    0.00 0   64.0648000    -296810.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10548.127
-5.310842140D+04 9.090311670D+02-2.356891244D+00 2.204449885D-02-2.510781471D-05
 1.446300484D-08-3.369070940D-12                -4.113752080D+04 4.045514860D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10548.127
-1.127640116D+05-8.252261380D+02 7.616178630D+00-1.999327610D-04 5.655631430D-08
-5.454316610D-12 2.918294102D-16                -3.351308690D+04-1.655773744D+01
SO2-            TPIS 1989 v1 pt1 p290;pt2 p176.
 2 tpis89 S   1.00O   2.00E   1.00    0.00    0.00 0   64.0653486    -408606.069
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10749.431
 9.460901660D+04-8.562691050D+02 5.360074220D+00 7.609576740D-03-1.092005659D-05
 7.202547730D-09-1.850138220D-12                -4.580094810D+04-3.929933190D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10749.431
-1.793400005D+05-3.663168760D+02 7.274441050D+00-1.101944663D-04 2.443328132D-08
-2.809735019D-12 1.305160431D-16                -4.973072610D+04-1.261418815D+01
SO2CLF
 2 J 6/71 S   1.00O   2.00CL  1.00F   1.00    0.00 0  118.5159032    -556475.704
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 2.981752800D+00 2.644916700D-02-2.920018200D-05
 1.395761100D-08-2.030448700D-12                -6.876149700D+04 1.273168120D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 1.011828600D+01 3.148899400D-03-1.347151400D-06
 2.558031000D-10-1.793825600D-14                -7.050929100D+04-2.312785080D+01
SO2CL2
 2 J 6/71 S   1.00O   2.00CL  2.00    0.00    0.00 0  134.9702000    -354802.065
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.385167700D+00 2.321215700D-02-2.653211200D-05
 1.349992300D-08-2.281928100D-12                -4.480297400D+04 6.578678800D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 1.055093700D+01 2.673430100D-03-1.142823000D-06
 2.168620000D-10-1.519915100D-14                -4.629505600D+04-2.430785700D+01
SO2F2           TPIS 1989 v1 pt1 p313;pt2 p193.
 2 tpis89 S   1.00O   2.00F   2.00    0.00    0.00 0  102.0616064    -760000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13490.451
 5.533191170D+04-8.074693970D+02 5.287203340D+00 2.294538400D-02-2.891010090D-05
 1.785619590D-08-4.418880790D-12                -8.899426230D+04-4.124413550D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13490.451
-3.403275690D+05-1.309477830D+03 1.396623280D+01-3.841301960D-04 8.460174630D-08
-9.683165050D-12 4.482704400D-16                -8.901873960D+04-5.109423950D+01
SO3             TPIS 1989 v1 pt1 p292;pt2 p177
 2 tpis89 S   1.00O   3.00    0.00    0.00    0.00 0   80.0642000    -395900.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11688.499
-3.953058420D+04 6.208856370D+02-1.437885220D+00 2.764167890D-02-3.145018200D-05
 1.792841690D-08-4.126515350D-12                -5.184119840D+04 3.391418860D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11688.499
-2.166404920D+05-1.301181450D+03 1.096306490D+01-3.838139080D-04 8.469871470D-08
-9.709594230D-12 4.500688030D-16                -4.398183130D+04-3.655347580D+01
S2              TPIS 1989 v1 pt1 p270;pt2 p165.
 2 tpis89 S   2.00    0.00    0.00    0.00    0.00 0   64.1320000     128600.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9132.110
 3.528091780D+04-4.222156580D+02 4.677433490D+00 1.724046361D-03-3.862208210D-06
 3.336156340D-09-9.930661540D-13                1.654767715D+04-7.956811240D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9132.110
-1.588128788D+04 6.315480880D+02 2.449628069D+00 1.986240565D-03-6.507927240D-07
 1.002813651D-10-5.596990050D-15                1.085508427D+04 1.458549193D+01
S2-             TPIS 1989 v1 pt1 p274;pt2 p166.
 2 tpis89 S   2.00E   1.00    0.00    0.00    0.00 0   64.1325486     -37132.385
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9597.115
 1.025558251D+04-6.166128250D+02 8.182052840D+00-8.311203580D-03 9.720274160D-06
-5.775476780D-09 1.393690695D-12                -3.063559874D+03-1.906063363D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9597.115
 4.830204030D+05-1.319171302D+03 6.031778480D+00-7.965560690D-04 2.282241690D-07
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-2.504364698D-11 7.280550780D-16                2.660258490D+03-9.010433540D+00
S2CL2
 2 G 4/93 S   2.00CL  2.00    0.00    0.00    0.00 0  135.0374000    -16736.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.479057080D+00 3.253700280D-02-6.639046200D-05
 6.211248450D-08-2.171123250D-11               -4.022255670D+03 1.227918240D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.468410200D+00 1.121863520D-03-6.927842800D-07
 1.386544630D-10-9.293978390D-15               -5.050195240D+03-1.529504410D+01
S2F2,thiothony    Thiothony fluoride. JPCRD 1985 sup1 v14 pt2 p1105.
 2 j 6/76 S   2.00F   2.00    0.00    0.00    0.00 0  102.1288064    -401413.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13717.892
 1.252904041D+05-1.941243874D+03 1.325382183D+01-1.341525124D-03-2.772465632D-06
 3.658169290D-09-1.299531209D-12 0.000000000D+00-4.067208250D+04-4.560825680D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13717.892
-2.591757719D+05-1.059653069D+02 1.006588551D+01-2.274618148D-05 5.412343140D-09
-9.911387140D-13 9.621861440D-17 0.000000000D+00-5.147675180D+04-2.375663203D+01
S2O             TPIS 1989 v1 pt1 p293;pt2 p178.
 2 tpis89 S   2.00O   1.00    0.00    0.00    0.00 0   80.1314000     -56035.495
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11128.557
 1.092703310D+04-9.523099870D+01 3.144525430D+00 1.176854200D-02-1.580266840D-05
 1.037645040D-08-2.708622260D-12               -7.500471900D+03 1.104173640D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11128.557
-1.442139790D+05-3.276430130D+02 7.244286110D+00-9.776538300D-05 2.162712700D-08
-2.482782220D-12 1.151778750D-16               -7.438553930D+03-1.085177000D+01
S3              TPIS 1989 v1 pt1 p275;pt2 p167.
 2 tpis89 S   3.00    0.00    0.00    0.00    0.00 0   96.1980000     144738.328
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11974.328
 7.245403660D+04-1.162148040D+03 9.955421730D+00-4.158052530D-03 3.241824490D-06
-1.264688430D-09 1.777585680D-13                2.146276070D+04-2.587525550D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11974.328
-1.117820100D+05-5.198656000D+01 7.038781910D+00-1.548573410D-05 3.415000930D-09
-3.908461800D-13 1.808437520D-17                1.525410080D+04-7.610137390D+00
S4              TPIS 1989 v1 pt1 p277;pt2 p168.
 2 tpis89 S   4.00    0.00    0.00    0.00    0.00 0  128.2640000     135632.333
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14280.333
 1.198673860D+05-2.040798720D+03 1.510240760D+01-7.041233260D-03 5.350555550D-06
-2.002433890D-09 2.570126320D-13                2.410915440D+04-5.503181360D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14280.333
-2.068585710D+05-9.688859620D+01 1.007234930D+01-2.890294000D-05 6.373344840D-09
-7.289735740D-13 3.369145170D-17                1.321062970D+04-2.344808450D+01
S5              TPIS 1989 v1 pt1 p281;pt2 p169.
 2 tpis89 S   5.00    0.00    0.00    0.00    0.00 0  160.3300000     132993.354
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19053.353
 1.361391360D+05-2.955502820D+03 2.633370960D+01-4.125833090D-02 7.056843570D-05
-5.611111760D-08 1.659460860D-11                2.675320050D+04-1.069717610D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19053.353
-4.038678250D+06 8.602287260D+03 7.443287440D+00 1.533644870D-03-2.533387560D-07
 2.146096100D-11-7.217671890D-16               -4.687238840D+04 1.104591840D+01
S6              TPIS 1989 v1 pt1 p282;pt2 p170.
 2 tpis89 S   6.00    0.00    0.00    0.00    0.00 0  192.3960000     101315.179
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22787.179
 9.782032260D+04-2.568715240D+03 2.467161180D+01-1.620360020D-02 1.712892680D-05
-9.750494040D-09 2.488221690D-12                2.038005970D+04-1.014485270D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22787.179
 3.686830920D+06-7.694976080D+03 1.860717690D+01 2.290403800D-03-1.219839720D-06
 2.060789030D-10-1.190359260D-14                6.032459600D+04-7.490209710D+01
S7              TPIS, vol 1 part 1,1989 p.277,283-284.
 2 tpis89 S   7.00    0.00    0.00    0.00    0.00 0  224.4620000     111890.368
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26274.368
 1.233582300D+05-3.200434880D+03 3.015616360D+01-2.197295540D-02 2.487632540D-05
-1.505861270D-08 3.768393330D-12                2.389954190D+04-1.275943120D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26274.368
-2.726989530D+05-7.355039380D+01 1.905750840D+01-2.382707030D-05 5.409245710D-09
-6.334770940D-13 2.985594150D-17                7.307306220D+03-6.158956790D+01
S8              TPIS 1989 v1 pt1 p284;pt2 p172.
 2 tpis89 S   8.00    0.00    0.00    0.00    0.00 0  256.5280000     101277.123
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31573.122
 3.145377840D+05-6.116163490D+03 4.875140130D+01-6.241291090D-02 7.421117820D-05
-3.725939830D-08 5.797988380D-12                3.573723870D+04-2.288596760D+02
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31573.122
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-8.728336090D+06 1.221738910D+04 2.209843410D+01-3.493451490D-03 1.397433300D-06
-2.169577930D-10 1.212176000D-14              -8.658828090D+04-6.434898620D+01
Sc            Hf0:TPIS v4 1982. Spec:JPCRD v14 sup2 1985.
 3 g 1/99 SC  1.00    0.00    0.00    0.00    0.00 0   44.9559100     377700.259
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7002.259
-3.700805940D+03 1.692506026D+02 1.842242597D+00 1.364835821D-03-1.580085847D-06
 9.613111150D-10-2.392381918D-13              4.385215240D+04 1.072781921D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7002.259
 8.810382650D+06-2.711232975D+04 3.476588660D+01-1.861104581D-02 5.290283900D-06
-6.585408060D-10 2.997850429D-14              2.162460097D+05-2.225618519D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7002.259
 2.283130511D+09-1.367701232D+06 3.213593060D+02-3.563171100D-02 2.093254715D-06
-6.238650020D-11 7.425605615D-16              1.092708359D+07-2.781409383D+03
Sc+           Levels:JPCRD v14 sup2 1985.
 3 g 7/97 SC  1.00E  -1.00    0.00    0.00    0.00 0   44.9553614    1017145.222
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7161.922
-5.884930160D+03 1.479044408D+02 2.009576456D+00 7.389566970D-04-6.617964820D-07
 6.841073760D-10-2.164125532D-13              1.208439139D+05 1.026570620D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7161.922
 1.973658531D+06-4.954384100D+03 6.360627350D+00-7.168785920D-04 2.464991123D-08
 9.632373790D-12-8.544709642D-16              1.543423764D+05-2.261925782D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7161.922
 2.219151811D+08-1.287881370D+05 3.265593870D+01-3.379963200D-03 1.981741972D-07
-5.190207160D-12 4.635586113D-17              1.149364313D+06-2.553294937D+02
Sc-           JPCRD v14 n3 1985 p731. Used J from isoelectronic Ti.
 3 g 9/97 SC  1.00E   1.00    0.00    0.00    0.00 0   44.9564586     352558.828
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              4.165746390D+04 8.270420720D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              4.165746390D+04 8.270420720D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              4.165746390D+04 8.270420720D+00
Si            Hf:CODATA1989. Levels:NIST data version1.1 [Online]1997.
 3 g 8/97 SI  1.00    0.00    0.00    0.00    0.00 0   28.0855000     450000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7550.258
 9.836140810D+01 1.546544523D+02 1.876436670D+00 1.320637995D-03-1.529720059D-06
 8.950562770D-10-1.952873490D-13              5.263510310D+04 9.698288880D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7550.258
-6.169298850D+05 2.240683927D+03-4.448619320D-01 1.710056321D-03-4.107714160D-07
 4.558884780D-11-1.889515353D-15              3.953558760D+04 2.679668061D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7550.258
-9.286548940D+08 5.443989890D+05-1.206739736D+02 1.359662698D-02-7.606498660D-07
 2.149746065D-11-2.474116774D-16             -4.293792120D+06 1.086382839D+03
Si+           JPCRD v12 n2 1983 p323.
 3 g 4/97 SI  1.00E  -1.00    0.00    0.00    0.00 0   28.0849514    1242508.045
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7342.945
-4.329791880D+04 6.795894490D+02 2.257046144D-01 4.118600490D-03-4.234881600D-06
 2.327995626D-09-5.318388059D-13              1.452039813D+05 1.934650510D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7342.945
 5.919390230D+04-4.856730950D+01 2.556312024D+00-3.503397160D-05 1.190298787D-08
-2.082923821D-12 1.471452049D-16              1.491431392D+05 5.244267140D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7342.945
-1.364223349D+07 7.022777180D+03 1.233010042D+00 1.211789390D-04-1.455223586D-08
 1.530293455D-12-3.804350544D-17              9.149238100D+04 1.708337812D+01
Si-           Spec: JANAF 3/83. EA:JPCRD v14 n3 1985 p731.
 3 g 4/97 SI  1.00E   1.00    0.00    0.00    0.00 0   28.0860486     308817.528
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-7.940146670D+02 5.567418420D+00 2.499837183D+00-9.481394460D-05 3.171246930D-07
-4.191323180D-10 2.035924380D-13              3.636443380D+04 5.270119840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-6.162070100D+06 1.883310402D+04-1.899302450D+01 1.111021657D-02-2.535790208D-06
 2.699962923D-10-1.105062911D-14             -8.314089310D+04 1.595298253D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-5.429517960D+07 3.297105700D+04-2.470579690D+00 3.966577600D-04-1.764141255D-08
 4.115769760D-13-3.904369380D-18             -2.315881505D+05 5.226601830D+01
SiBr          D0,Props: TPIS 1991 V2 pt1 p280; pt2 p249.
 2 tpis91 SI  1.00BR  1.00    0.00    0.00    0.00 0  107.9895000     175157.421
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10035.121
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 7.370283350D+03-5.051062960D+02 8.280591040D+00-1.005383920D-02 1.357050920D-05
-9.115449900D-09 2.447477685D-12              2.184405475D+04-1.662032657D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10035.121
 1.317799940D+06-3.669795020D+03 8.511686120D+00-1.987602041D-03 5.035414890D-07
-4.490120190D-11 8.235670070D-16              4.332851550D+04-2.467075472D+01
SiBr2           TPIS 1991 V2 pt1 p281; pt2 p250.
 2 tpis91 SI  1.00BR  2.00    0.00    0.00    0.00 0  187.8935000     -51000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13317.161
 2.386344840D+04-6.415309660D+02 9.345668330D+00-4.792326090D-03 5.581697420D-06
-3.454694230D-09 8.798534250D-13              -5.014941350D+03-1.740650160D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13317.161
-5.143438210D+04-1.291344250D+01 7.010376190D+00-4.400447250D-06 1.018929130D-09
-1.212967970D-13 5.792398720D-18              -8.318693430D+03-3.613055220D+00
SiBr3           TPIS 1991 V2 pt1 p282; pt2 p251.
 2 tpis91 SI  1.00BR  3.00    0.00    0.00    0.00 0  267.7975000    -157000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17461.439
 3.973369990D+04-1.066545780D+03 1.380868960D+01-7.641812890D-03 8.776554710D-06
-5.372681400D-09 1.356451040D-12              -1.651760630D+04-3.784244450D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17461.439
-8.888495900D+04-2.267361090D+01 1.001791580D+01-7.488719070D-06 1.712641640D-09
-2.017512570D-13 9.550866230D-18              -2.203031110D+04-1.537576360D+01
SiBr4           TPIS 1991 V2 pt1 p283; pt2 p252.
 2 tpis91 SI  1.00BR  4.00    0.00    0.00    0.00 0  347.7015000    -415800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22313.721
 6.819815960D+04-1.520182720D+03 1.810344060D+01-9.731475380D-03 1.071861150D-05
-6.339802640D-09 1.555939560D-12              -4.616674580D+04-5.975518610D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22313.721
-1.273177830D+05-3.719168090D+01 1.302857710D+01-1.166200630D-05 2.611298180D-09
-3.018865710D-13 1.405382690D-17              -5.409313420D+04-2.940003680D+01
SiC             Hf0,Props: TPIS 1991 V2 pt1 p301; pt2 p265.
 2 tpis91 SI  1.00C   1.00    0.00    0.00    0.00 0   40.0962000     734946.140
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9217.111
-6.223330890D+03 3.141790457D+02 3.893130830D-01 1.187507540D-02-1.639277197D-05
 1.131808223D-08-3.045324231D-12               8.606227730D+04 2.310164473D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9217.111
-6.268806030D+04 7.209836920D+02 2.162879732D+00 2.201299585D-03-6.569466590D-07
 9.177110260D-11-4.969166740D-15               8.321225850D+04 1.601673073D+01
SiC2            TPIS, vol 2, part 1,1991 p246,302-4.
 2 tpis91 SI  1.00C   2.00    0.00    0.00    0.00 0   52.1069000     631360.938
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11685.409
-4.119658400D+04 6.869790750D+02 2.358756990D-02 1.532947120D-02-1.435601900D-05
 6.375338600D-09-1.059241670D-12               7.130888640D+04 2.828862756D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11685.409
 7.026787990D+06-2.466118590D+04 3.915420320D+01-2.002866430D-02 6.307304410D-06
-8.848315380D-10 4.530513160D-14               2.267306020D+05-2.366598676D+02
SiC4H12
 2 J12/60 SI  1.00C   4.00H  12.00    0.00    0.00 0   88.2235800    -286604.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.946186260D+00 4.114297430D-02-2.932337420D-07
-2.290036940D-08 1.095667730D-11              -3.773104920D+04 3.186270184D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.156370180D+01 3.281120640D-02-1.263708910D-05
 2.268685110D-09-1.542694770D-13              -4.013813660D+04-3.363416030D+01
SiCL            TPIS, vol 2, part 1,1989 p258,271-73.
 2 g 7/95 SI  1.00CL  1.00    0.00    0.00    0.00 0   63.5382000     142360.251
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9881.277
 1.346763490D+04-2.170490740D+02 5.034083020D+00-6.567498940D-04 4.839472130D-07
-1.400176870D-10 4.311131910D-15               1.692801150D+04-5.641114140D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9881.277
-2.571614660D+05 7.292136980D+02 3.602449110D+00 5.932771920D-04-1.694267230D-07
 2.474390020D-11-1.103378870D-15               1.110513490D+04 9.159306480D+00
SiCL2           TPIS 1991 v2 pt1 p273; pt2 p244.
 2 tpis91 SI  1.00CL  2.00    0.00    0.00    0.00 0   98.9909000    -163069.287
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12529.294
 5.305144050D+04-1.015782150D+03 1.032812830D+01-6.211234950D-03 6.714227620D-06
-3.907553480D-09 9.457868190D-13              -1.650246880D+04-2.649731900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12529.294
-8.048685550D+04-2.668970290D+01 7.020520120D+00-8.401992250D-06 1.892129420D-09
-2.204032970D-13 1.035131570D-17              -2.181245670D+04-6.639513170D+00
SiCL3           TPIS 1991 v2 pt1 p275; pt2 p245.
 2 tpis91 SI  1.00CL  3.00    0.00    0.00    0.00 0  134.4436000    -336271.671
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15717.466
 8.690861840D+04-1.677432020D+03 1.511447350D+01-8.934979170D-03 9.094262700D-06
-5.012242790D-09 1.155264560D-12                -3.477536710D+04-5.086820230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15717.466
-1.476977780D+05-5.342570450D+01 1.004053900D+01-1.642237280D-05 3.666693190D-09
-4.241786280D-13 1.981070140D-17                -4.360526260D+04-2.006705460D+01
SiCL4           TPIS 1991 v2 pt1 p276; pt2 p246.
 2 tpis91 SI  1.00CL  4.00    0.00    0.00    0.00 0  169.8963000    -662200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19455.437
 1.171752360D+05-2.185973620D+03 1.908336020D+01-9.638765240D-03 8.840541810D-06
-4.362893810D-09 8.948968160D-13                -7.212729300D+04-7.302007270D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19455.437
-2.102535760D+05-8.415230880D+01 1.306300030D+01-2.521203220D-05 5.566817410D-09
-6.374061120D-13 2.948581540D-17                -8.372660480D+04-3.592122790D+01
SiF             TPIS 1991 v2 pt1 p264; pt2 p238.
 2 g 3/99 SI  1.00F   1.00    0.00    0.00    0.00 0   47.0839032     -25231.846
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9456.954
 1.343519512D+04 3.341196970D+01 2.209142264D+00 7.455340730D-03-1.072510181D-05
 7.515362000D-09-2.071774483D-12                -4.089122740D+03 1.294598349D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9456.954
-1.809808236D+05 2.897332358D+02 4.102863560D+00 2.873698120D-04-8.052869220D-08
 1.186380657D-11-5.050512920D-16                -6.450449550D+03 3.852766520D+00
SiFCL           TPIS, vol 2, part 1,1991 p260,279-80.
 2 tpis91 SI  1.00F   1.00CL  1.00    0.00    0.00 0   82.5366032    -377825.696
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11832.883
 4.177080110D+04-5.926760410D+02 6.409877350D+00 4.641373320D-03-7.977985560D-06
 6.008358670D-09-1.720839940D-12                -4.398277400D+04-6.260331480D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11832.883
-1.284615390D+05-1.247806040D+02 7.092922270D+00-3.708753890D-05 8.178794290D-09
-9.360815140D-13 4.330581560D-17                -4.723283570D+04-8.337603240D+00
SiF2            TPIS 1991 v2  pt1 p266; pt2 p239.
 2 tpis91 SI  1.00F   2.00    0.00    0.00    0.00 0   66.0823064    -592838.108
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11204.470
 4.053035490D+04-3.997343870D+02 4.055135290D+00 1.153471970D-02-1.757662690D-05
 1.260428910D-08-3.517291870D-12                -7.047784460D+04 3.880785120D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11204.470
-1.675296440D+05-1.845976920D+02 7.136965970D+00-5.450046130D-05 1.198936930D-08
-1.369550340D-12 6.326305300D-17                -7.287416530D+04-1.117918090D+01
SiF3            TPIS 1991 v2 pt1 p268; pt2 p240
 2 tpis91 SI  1.00F   3.00    0.00    0.00    0.00 0   85.0807096    -996436.577
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13018.554
 5.755096030D+04-7.179211630D+02 5.379186280D+00 1.813123550D-02-2.738460640D-05
 1.946586450D-08-5.390996660D-12                -1.177633020D+05-3.441729220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13018.554
-2.903658550D+05-3.426807650D+02 1.025524670D+01-1.019182900D-04 2.248695080D-08
-2.575024740D-12 1.191898300D-16                -1.218095820D+05-2.725177150D+01
SiF4            TPIS 1991 v2 pt1 p269; pt2 p241.
 2 tpis91 SI  1.00F   4.00    0.00    0.00    0.00 0  104.0791128   -1615000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15355.893
 1.240774080D+04-1.235787460D+02 2.683003450D+00 3.267354470D-02-4.553162250D-05
 3.085537440D-08-8.267170450D-12                -1.954000070D+05 1.040294500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15355.893
-3.873748800D+05-6.296781370D+02 1.347017040D+01-1.882395490D-04 4.163775260D-08
-4.778712680D-12 2.216195340D-16                -1.957895810D+05-4.652313170D+01
SiH             TPIS 1991 v2 pt1 p257; pt2 p234.
 2 g 3/99 SI  1.00H   1.00    0.00    0.00    0.00 0   29.0934400     368718.358
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9227.258
-2.665600539D+03 2.924611327D+01 4.210147080D+00-4.780124130D-03 1.112230898D-05
-9.231694670D-09 2.747627561D-12                4.304668730D+04 9.211330230D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9227.258
-1.470883237D+06 3.710035090D+03-8.805991990D-02 2.375295836D-03-4.781914160D-07
 4.839908100D-11-1.750128856D-15                1.896966276D+04 2.979758536D+01
SiH+
 2 J12/71 SI  1.00H   1.00E  -1.00    0.00    0.00 0   29.0928914    1147699.773
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.729258800D+00-1.788161100D-03 4.246925700D-06
-2.558013000D-09 4.063374000D-13                1.369707100D+05 1.583873140D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.982859500D+00 1.545522200D-03-5.903855500D-07
 1.051740000D-10-6.822023400D-15                1.370795400D+05 5.040350140D+00
SiHBr3
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 2 J12/76 SI  1.00H   1.00BR  3.00    0.00    0.00 0  268.8054400    -302927.675
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.337011000D+00 2.887299000D-02-4.695412000D-05
 3.752303800D-08-1.163491900D-11               -3.866383400D+04 1.032167120D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.027483100D+01 2.866610400D-03-1.211258100D-06
 2.300491600D-10-1.623350400D-14               -3.984657600D+04-1.803406580D+01
SiHCL           TPIS 1991 v2 pt1 p277; pt2 p247.
 2 tpis91 SI  1.00H   1.00CL  1.00    0.00    0.00 0   64.5461400      54945.913
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10665.413
 5.909673050D+04-8.780064030D+02 7.999687930D+00-4.663141270D-03 8.594986000D-06
-6.608073550D-09 1.868076396D-12               9.567570340D+03-1.690015008D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10665.413
 1.012152890D+05-1.163239598D+03 7.376366550D+00 1.874151313D-04-1.661351093D-07
 3.964414040D-11-2.640580080D-15               1.141064087D+04-1.507679495D+01
SiHCL3
 2 J12/76 SI  1.00H   1.00CL  3.00    0.00    0.00 0  135.4515400    -496233.684
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.674204200D+00 3.438038500D-02-5.495385600D-05
 4.310333200D-08-1.315701200D-11               -6.160172300D+04 1.433350950D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.933563500D+00 3.248122000D-03-1.378717100D-06
 2.626607300D-10-1.857488600D-14               -6.307084900D+04-2.047205850D+01
SiHF            TPIS 1991 v2 pt1 p270; pt2 p242.
 2 tpis91 SI  1.00H   1.00F   1.00    0.00    0.00 0   48.0918432    -162657.169
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10230.231
 2.192598671D+04-6.175229080D+01 2.127372739D+00 1.123538312D-02-1.322503985D-05
 8.307307390D-09-2.010545971D-12               -2.016994845D+04 1.367184876D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10230.231
 4.049752240D+06-9.295526820D+03 1.071754366D+01 1.868124220D-03-1.129820372D-06
 1.960250100D-10-1.144682011D-14               4.133225200D+04-4.736317600D+01
SiHF3
 2 J 6/76 SI  1.00H   1.00F   3.00    0.00    0.00 0   86.0886496   -1200839.727
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.065481600D-01 3.326526700D-02-4.392882500D-05
 2.932836700D-08-7.864918800D-12               -1.458419600D+05 1.997326570D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.754882800D+00 4.552775600D-03-1.947753100D-06
 3.730079400D-10-2.647397300D-14               -1.476565800D+05-1.882697730D+01
SiHI3
 2 J12/76 SI  1.00H   1.00I   3.00    0.00    0.00 0  409.8068500     -74475.337
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.521122500D+00 2.484105400D-02-4.083398400D-05
 3.306839300D-08-1.037377400D-11               -1.140718900D+04 7.784669510D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.053360400D+01 2.588800000D-03-1.092190300D-06
 2.072068700D-10-1.460985400D-14               -1.239734500D+04-1.609503420D+01
SiH2            TPIS 1991 v2 pt1 p260; pt2 p235.
 2 g 3/99 SI  1.00H   2.00    0.00    0.00    0.00 0   30.1013800     273350.215
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10035.788
-1.958341120D+05 2.758775006D+03-9.908961010D+00 2.763174564D-02-1.030655393D-05
-9.050659080D-09 5.892700820D-12               1.833344160D+04 8.185889390D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10035.788
-2.005373278D+06 3.817563320D+03 4.158125620D+00 1.034977640D-03-2.058047054D-07
 2.278901963D-11-1.064318464D-15               3.984823830D+03 4.836272660D+00
SiH2Br2
 2 J12/76 SI  1.00H   2.00BR  2.00    0.00    0.00 0  189.9093800    -190375.706
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.000742700D+00 3.028263100D-02-4.468733600D-05
 3.441143100D-08-1.054872000D-11               -2.450750700D+04 1.856673660D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.169260100D+00 5.028560100D-03-2.109756400D-06
 3.987215500D-10-2.803583800D-14               -2.584247500D+04-1.137119140D+01
SiH2CL2
 2 J12/76 SI  1.00H   2.00CL  2.00    0.00    0.00 0  101.0067800    -320501.804
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.026493800D+00 3.301358900D-02-4.796106200D-05
 3.622567600D-08-1.092044700D-11               -3.996338700D+04 2.062885730D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.912140400D+00 5.312789100D-03-2.233672900D-06
 4.227481200D-10-2.975568400D-14               -4.146850300D+04-1.288676270D+01
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SiH2F2
 2 J 6/76 SI  1.00H   2.00F   2.00    0.00    0.00 0   68.0981864    -790797.565
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.937599800D-01 3.007988000D-02-3.587413600D-05
 2.266855800D-08-5.918592500D-12              -9.623032700D+04 2.286075360D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.098185700D+00 6.214649000D-03-2.627235200D-06
 4.990908500D-10-3.522164100D-14              -9.791874500D+04-1.167256940D+01
SiH2I2
 2 J12/76 SI  1.00H   2.00I   2.00    0.00    0.00 0  283.9103200     -38073.923
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.656281300D+00 2.862617600D-02-4.300370000D-05
 3.370803100D-08-1.047554700D-11              -6.325261200D+03 1.727092510D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.357309900D+00 4.816358600D-03-2.016144500D-06
 3.804369900D-10-2.672058400D-14              -7.541766700D+03-1.029735490D+01
SiH3            TPIS 1991 v2 pt1 p261; pt2 p236.
 2 g 3/99 SI  1.00H   3.00    0.00    0.00    0.00 0   31.1093200     204357.366
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10276.989
 4.341142820D+03 2.277185085D+02 6.508250350D-01 1.221438558D-02-4.347604270D-06
-1.774916828D-09 1.184191367D-12               2.259993826D+04 1.968347482D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10276.989
 6.056321220D+05-4.721254060D+03 1.329129523D+01-1.256824868D-03 2.688285940D-07
-3.010741582D-11 1.370945857D-15               4.974420640D+04-6.140503100D+01
SiH3Br
 2 J12/76 SI  1.00H   3.00BR  1.00    0.00    0.00 0  111.0133200     -78242.643
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.006033500D+00 2.530787600D-02-3.039643300D-05
 2.108215000D-08-6.205539800D-12              -1.060536000D+04 1.946754460D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.135036300D+00 7.111291400D-03-2.973507500D-06
 5.606185700D-10-3.935084700D-14              -1.187990000D+04-6.178265690D+00
SiH3CL
 2 J12/76 SI  1.00H   3.00CL  1.00    0.00    0.00 0   66.5620200    -141841.392
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.830798500D-01 2.616172800D-02-3.085407300D-05
 2.087839500D-08-6.015367800D-12              -1.816197900D+04 2.023653790D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.991971800D+00 7.271893800D-03-3.044159000D-06
 5.743962000D-10-4.034092900D-14              -1.951493000D+04-6.867643670D+00
SiH3F
 2 J 6/76 SI  1.00H   3.00F   1.00    0.00    0.00 0   50.1077232    -376571.110
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.736972600D-01 2.337103600D-02-2.192597300D-05
 1.143866800D-08-2.621759800D-12              -4.626867600D+04 2.045412980D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.573611900D+00 7.741007500D-03-3.250275800D-06
 6.145479200D-10-4.322377400D-14              -4.768848600D+04-6.210022920D+00
SiH3I
 2 J12/76 SI  1.00H   3.00I   1.00    0.00    0.00 0  158.0137900      -2091.662
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.365932000D+00 2.459257500D-02-2.999179500D-05
 2.121514300D-08-6.348297100D-12              -1.525835500D+03 1.864039790D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.268666300D+00 6.965230500D-03-2.910274000D-06
 5.484146700D-10-3.848008800D-14              -2.737352700D+03-5.828451560D+00
SiH4            Silane. TPIS 1991 v2 pt1 p263 pt 2 p237.
 2 tpis91 SI  1.00H   4.00    0.00    0.00    0.00 0   32.1172600      34700.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10535.001
 7.873074590D+04-5.526220910D+02 2.499029280D+00 1.442091870D-02-8.466686240D-06
 2.725836390D-09-5.435770580D-13               6.269731340D+03 4.965000050D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10535.001
 1.290384930D+06-7.813430760D+03 1.828856250D+01-1.975650520D-03 4.156596000D-07
-4.596888580D-11 2.072860150D-15               4.766906570D+04-9.801729420D+01
SiI             TPIS 1991 v2 pt1 p284; pt2 p253.
 2 g 3/99 SI  1.00I   1.00    0.00    0.00    0.00 0  154.9899700     262953.589
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9941.289
 9.661426720D+04-1.598808950D+03 1.252070970D+01-1.633868342D-02 1.751118145D-05
-9.660537570D-09 2.177300408D-12               3.791578840D+04-4.144801710D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9941.289
-3.442030910D+05 1.314266301D+03 3.142334141D+00 7.506663480D-04-1.670899956D-07
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 9.947637410D-12 1.854543957D-15              2.209608580D+04 1.509832510D+01
SiI2
 2 J12/77 SI  1.00I   2.00    0.00    0.00    0.00 0  281.8944400     92470.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.321551050D+00 1.442733800D-02-3.105176470D-05
 2.983192860D-08-1.057854730D-11              9.412182020D+03 1.081785670D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.743118550D+00 3.619831560D-04-1.952786440D-07
 4.358232010D-11-2.899867920D-15              9.069753640D+03 1.290972130D-02
SiN            TPIS 1991 V2 pt1 p295; pt2 p261.
 2 g 5/99 SI  1.00N   1.00    0.00    0.00    0.00 0   42.0922400    403668.437
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       8736.137
-1.464672152D+04 1.374993497D+02 3.678508580D+00-6.158499200D-03 2.309417067D-05
-2.294461481D-08 7.395665680D-12              4.673212990D+04 6.494565540D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       8736.137
-2.932685132D+06 5.853688590D+03 1.321451677D+00 1.258329284D-03-3.773886360D-07
 6.887761040D-11-4.189842590D-15              6.527148810D+03 2.553145875D+01
SiO            Hf0,Props: TPIS 1991 V2 pt1 p247; pt2 p227
 2 tpis91 SI  1.00O   1.00    0.00    0.00    0.00 0   44.0849000    -98842.418
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       8715.105
-4.722771050D+04 8.063137640D+02-1.636976133D+00 1.454275546D-02-1.723202046D-05
 1.042397340D-08-2.559365273D-12              -1.666585903D+04 3.355795700D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       8715.105
-1.765134162D+05-3.199177090D+01 4.477441930D+00 4.591764710D-06 3.558143150D-08
-1.327012559D-11 1.613253297D-15              -1.350842360D+04-8.386957330D-01
SiO2            TPIS 1991 V2 pt1 p256; pt2 p233.
 2 tpis91 SI  1.00O   2.00    0.00    0.00    0.00 0   60.0843000   -322073.477
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      10542.523
-3.362948780D+04 4.734078920D+02 2.309770671D-01 1.850230806D-02-2.242786671D-05
 1.364981554D-08-3.351935030D-12              -4.226487490D+04 2.295803206D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      10542.523
-1.464031193D+05-6.261441060D+02 7.964563710D+00-1.854119096D-04 4.095214670D-08
-4.697206760D-12 2.178054280D-16              -3.791834770D+04-2.045285414D+01
SiS            TPIS 1991 v2 pt1 p290; pt2 p258.
 2 tpis91 SI  1.00S   1.00    0.00    0.00    0.00 0   60.1515000    108194.407
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       8932.107
 3.599449290D+04-4.239723300D+02 4.654014420D+00 1.588470782D-03-3.310254360D-06
 2.706096479D-09-8.113517820D-13              1.411515571D+04-1.183176921D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       8932.107
-2.102323897D+06 6.228836180D+03-3.004120882D+00 4.495499930D-03-1.368821364D-06
 1.998097253D-10-9.882035800D-15              -2.795538166D+04 5.405831280D+01
SiS2            TPIS 1991 v2 pt1 p294; pt2 p260.
 2 tpis91 SI  1.00S   2.00    0.00    0.00    0.00 0   92.2175000      7022.717
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12203.217
 4.397745660D+04-7.430013120D+02 7.941588360D+00 2.038083730D-03-4.646337600D-06
 3.848014360D-09-1.157260149D-12              2.801077853D+03-1.736885072D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12203.217
-1.266489071D+05-9.774235220D+01 7.572803680D+00-2.905413928D-05 6.405587840D-09
-7.329273340D-13 3.389819780D-17              -1.244672263D+03-1.352707210D+01
Si2            TPIS 1991 v2 pt1 p240; pt2 p225.
 2 tpis91 SI  2.00    0.00    0.00    0.00    0.00 0   56.1710000    580195.524
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      10296.124
 1.237596221D+04-1.024904376D+02 4.354848520D+00 1.281063335D-03-2.531991623D-06
 2.265694244D-09-7.001290140D-13              6.906942850D+04 3.251125200D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      10296.124
 1.370060657D+06-4.207060040D+03 9.337432890D+00-2.749217168D-03 9.586345960D-07
-1.372449748D-10 6.765028100D-15              9.510884540D+04-3.168385190D+01
Si2C            TPIS 1991 V2 pt1 p304; pt2 p267.
 2 tpis91 SI  2.00C   1.00    0.00    0.00    0.00 0   68.1817000    554093.904
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      11582.346
-4.553612390D+03 1.314823390D+02 2.469097300D+00 1.276521680D-02-1.656909660D-05
 1.065286890D-08-2.739179190D-12              6.470048540D+04 1.468844240D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      11582.346
-1.254366580D+05-3.412746870D+02 7.254196690D+00-1.016717690D-04 2.248300890D-08
-2.580421640D-12 1.196883820D-16              6.607911310D+04-1.146096130D+01
Si2N
 2 J 3/67 SI  2.00N   1.00    0.00    0.00    0.00 0   70.1777400    397494.514
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.668673500D+00 1.130184000D-02-1.363711900D-05
 7.168805000D-09-1.237831000D-12              4.631808300D+04 7.122709640D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
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 0.000000000D+00 0.000000000D+00 6.670991200D+00 9.191788200D-04-3.951713000D-07
 7.439714500D-11-5.028469100D-15                4.562015400D+04-7.798277660D+00
Si3             TPIS 1991 V2 pt1 p246; pt2 p226.
 2 g 7/95 SI  3.00    0.00    0.00    0.00    0.00 0   84.2565000     627867.380
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12519.793
-1.114294410D+04 1.575910160D+02 2.486067470D+00 1.631654520D-02-2.208261330D-05
 1.372019790D-08-3.262348720D-12                7.328247890D+04 1.588119200D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        12519.793
-1.699325750D+06 4.697615260D+03 2.618421140D+00 1.958959790D-03-2.580813230D-07
 6.098565850D-12 6.088986530D-16                4.278044800D+04 2.586380450D+01
Sn              Hf:CODATA 1989 p24. NSRDS-NBS 35 vIII 1971 p74
 3 g 7/97 SN  1.00    0.00    0.00    0.00    0.00 0  118.7100000     301200.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6214.713
-1.248692263D+05 1.618841190D+03-4.602397350D+00 1.045433308D-02 2.998265550D-06
-1.068699386D-08 4.323421310D-12                2.748364008D+04 4.805067230D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6214.713
-5.145695640D+06 1.140575108D+04-4.179632060D+00 2.236390679D-03-3.603219770D-07
 2.440237836D-11-2.937628285D-16               -4.215013570D+04 5.981450930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6214.713
-1.119787114D+09 6.427046040D+05-1.378615913D+02 1.453867222D-02-7.109586030D-07
 1.501409263D-11-8.940758657D-17               -5.111296870D+06 1.245625545D+03
Sn+             NSRDS,NBS 35 vIII 1971 p80
 3 g 7/97 SN  1.00E  -1.00    0.00    0.00    0.00 0  118.7094514    1015949.928
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
-5.571297780D+03 1.222323189D+02 1.566361415D+00 3.397061410D-03-6.312922290D-06
 5.585452080D-09-1.689021340D-12                1.209024120D+05 1.162634765D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 4.622916850D+06-1.185958712D+04 1.237026473D+01-2.773624217D-03 3.098513490D-07
-5.362951440D-12-8.663474691D-16                1.994322977D+05-6.837108280D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6197.428
 1.913728057D+08-1.145730242D+05 3.070294184D+01-3.387878800D-03 1.966377351D-07
-4.388396290D-12 2.057062343D-17                1.031631149D+06-2.370157923D+02
Sn-             JPCRD v14 n3 1985 p731.
 3 g 9/97 SN  1.00E   1.00    0.00    0.00    0.00 0  118.7105486     179495.949
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6490.449
 2.722796000D+05-3.369935800D+03 1.743906405D+01-2.810527618D-02 2.790684767D-05
-1.442400675D-08 3.070159757D-12                3.753227750D+04-8.007856970D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6490.449
-6.447713220D+04 7.430555100D+02 1.921380256D+00 2.361623997D-04-5.280668360D-08
 6.102339380D-12-2.843422486D-16                1.645739414D+04 1.265436865D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6490.449
-1.314284778D+06 8.972354270D+02 2.302354538D+00 2.246840970D-05-1.392571963D-09
 4.468904450D-14-5.811846560D-19                1.428800599D+04 1.004933765D+01
SnBr            D0,props: TPIS 1991 V2 pt1 p378; pt2 p321.
 2 tpis91 SN  1.00BR  1.00    0.00    0.00    0.00 0    198.61400      75644.020
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9986.120
 2.564193542D+04-5.259122330D+02 7.687410690D+00-9.654205420D-03 1.482863248D-05
-9.942236980D-09 2.475051091D-12 0.000000000D+00 1.020483889D+04-1.126550396D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9986.120
 1.815578541D+06-6.728264580D+03 1.332464516D+01-4.608102300D-03 1.236439537D-06
-1.528863587D-10 6.971513500D-15 0.000000000D+00 4.925583090D+04-5.640962780D+01
SnBr2           TPIS 1991 v2 pt1 p380; pt2 p323.
 2 tpis91 SN  1.00BR  2.00    0.00    0.00    0.00 0  278.5180000    -118974.592
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14595.408
-4.995753060D+03-1.366498896D+02 7.543563850D+00-1.181772507D-03 1.442445852D-06
-9.254217260D-10 2.423731634D-13               -1.575506969D+04-3.595584020D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14595.408
-1.940894091D+04-2.335607932D+00 7.001969260D+00-8.622241870D-07 2.039869794D-10
-2.464780359D-14 1.189850894D-18               -1.644828122D+04-4.349354750D-01
SnBr3           TPIS 1991 v2 pt1 p381; pt2 p324.
 2 tpis91 SN  1.00BR  3.00    0.00    0.00    0.00 0  358.4220000    -158716.446
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19280.454
-8.050416470D+03-2.897962523D+02 1.114443355D+01-2.475383807D-03 3.010051350D-06
-1.925695320D-09 5.032605090D-13               -2.070066649D+04-1.895965383D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19280.454
-3.893004530D+04-4.990844170D+00 1.000418437D+01-1.824996910D-06 4.305646660D-10
-5.191887930D-14 2.502455595D-18               -2.217299473D+04-1.229854098D+01
SnBr4           TPIS 1991 v2 pt1 p384; pt2 p326.
 2 tpis91 SN  1.00BR  4.00    0.00    0.00    0.00 0  438.3260000    -324216.982
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25043.018
-5.832840920D+03-4.270198470D+02 1.467466525D+01-3.604263230D-03 4.366686290D-06
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-2.785875130D-09 7.265087870D-13              -4.082916450D+04-3.447104360D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       25043.018
-5.176812920D+04-7.426126950D+00 1.300619502D+01-2.692587978D-06 6.336759800D-10
-7.627087190D-14 3.671112000D-18              -4.300166340D+04-2.471455118D+01
SnCL            D0,Props: TPIS 1991 V2 pt1 p370; pt2 p315.
 2 tpis91 SN  1.00CL  1.00    0.00    0.00    0.00 0    154.16270      34658.816
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9644.116
 3.351549730D+04-6.832208620D+02 8.393917730D+00-1.164434373D-02 1.812159499D-05
-1.261999170D-08 3.295213470D-12 0.000000000D+00 6.051790890D+03-1.667834870D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9644.116
 7.741605680D+05-3.602048480D+03 9.749059820D+00-2.596198909D-03 6.367712160D-07
-6.754295570D-11 2.484167602D-15 0.000000000D+00 2.442447662D+04-3.225454390D+01
SnCL2           TPIS 1991 v2 pt1 p373; pt2 p317.
 2 tpis91 SN  1.00CL  2.00    0.00    0.00    0.00 0  189.6154000    -202648.283
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13681.717
 9.524665900D+03-4.329845640D+02 8.644720280D+00-3.458409610D-03 4.117852030D-06
-2.592639269D-09 6.692363600D-13              -2.432921127D+04-1.299144326D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13681.717
-3.903588490D+04-7.947962680D+00 7.006487620D+00-2.776594714D-06 6.461341420D-10
-7.119067400D-15 3.688131180D-18              -2.654529653D+04-3.368085920D+00
SnCL3           TPIS 1991 v2 pt1 p374; pt2 p318.
 2 tpis91 SN  1.00CL  3.00    0.00    0.00    0.00 0  225.0681000    -292372.455
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17554.045
 1.760076813D+04-8.142805480D+02 1.306326984D+01-6.395596190D-03 7.574624570D-06
-4.749711460D-09 1.222182656D-12              -3.413430960D+04-3.457680270D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17554.045
-7.482966400D+04-1.528523914D+01 1.001240305D+01-5.285581240D-06 1.226095111D-09
-1.459895108D-13 6.968879780D-18              -3.830878270D+04-1.663063737D+01
SnCL4           TPIS 1991 v2 pt1 p376; pt2 p320.
 2 tpis91 SN  1.00CL  4.00    0.00    0.00    0.00 0  260.5208000    -478465.969
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22474.031
 4.245967870D+04-1.280574318D+03 1.768445328D+01-9.574779520D-03 1.115620323D-05
-6.907229270D-09 1.759652856D-12              -5.504009040D+04-5.827353690D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22474.031
-1.078336862D+05-2.554305872D+01 1.302040391D+01-8.595125900D-06 1.976570888D-09
-2.337929994D-13 1.110287624D-17              -6.163562030D+04-3.072703313D+01
SnF             D0,Props: TPIS 1991 v2 pt1 p365; pt2 p310.
 2 tpis91 SN  1.00F   1.00    0.00    0.00    0.00 0  137.7084032     -95017.090
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9136.110
 6.098503520D+04-9.860306290D+02 8.994731210D+00-1.223012156D-02 1.840583578D-05
-1.267926607D-08 3.291331020D-12              -7.882614480D+03-2.221921734D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9136.110
 2.589715476D+04-1.484478214D+03 7.378518930D+00-1.324244440D-03 2.847634043D-07
-2.360371345D-11 6.116783710D-16              -4.776688970D+03-1.681202516D+01
SnF2            TPIS 1991 v2 pt1 p368; pt2 p312.
 2 tpis91 SN  1.00F   2.00    0.00    0.00    0.00 0  156.7068064    -510956.951
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12243.049
 7.042391850D+04-1.137505955D+03 1.008659352D+01-4.722855930D-03 4.135702920D-06
-1.921143972D-09 3.640760280D-13              -5.756670820D+04-2.571566624D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12243.049
-1.027758772D+05-4.451751620D+01 7.033268760D+00-1.329882797D-05 2.934271938D-09
-3.358415920D-13 1.553358669D-17              -6.362125880D+04-6.810084520D+00
SnF3            TPIS 1991 v2 pt1 p369; pt2 p313.
 2 tpis91 SN  1.00F   3.00    0.00    0.00    0.00 0  175.7052096    -646630.479
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14799.721
 1.095555529D+05-1.950557979D+03 1.541407832D+01-8.546518770D-03 7.800551820D-06
-3.825942220D-09 7.787747760D-13              -7.056794920D+04-5.494639480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14799.721
-1.829319689D+05-7.557358680D+01 1.005671455D+01-2.275132668D-05 5.034695820D-09
-5.776530960D-13 2.677214170D-17              -8.091897590D+04-2.191673972D+01
SnF4            TPIS 1991 v2 pt1 p369; pt2 p314.
 2 tpis91 SN  1.00F   4.00    0.00    0.00    0.00 0  194.7036128   -1024766.717
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18801.983
 1.390441119D+05-2.168784371D+03 1.691802917D+01-2.318608529D-03-2.045847976D-06
 3.430087900D-09-1.289228860D-12              -1.153563396D+05-6.370604750D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18801.983
-2.635692764D+05-1.445469969D+02 1.310690681D+01-4.237755790D-05 9.286871950D-09
-1.057062694D-12 4.867108680D-17              -1.271539967D+05-3.803921900D+01
SnI             D0,Props: TPIS 1991 V2 pt1 p384; pt2 p327.
 2 tpis91 SN  1.00I   1.00    0.00    0.00    0.00 0    245.61447     172725.022
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10177.122
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 2.670212235D+04-5.006026350D+02 7.490673150D+00-8.746346550D-03 1.289688397D-05
-8.211344930D-09 1.936120475D-12 0.000000000D+00 2.177249172D+04-9.354806850D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10177.122
-5.554991850D+04-1.530457453D+03 7.932601390D+00-2.108885464D-03 7.809803600D-07
-1.348104887D-10 8.207184700D-15 0.000000000D+00 2.744864953D+04-1.626822892D+01
SnI2            TPIS 1991 v2 pt1 p387; pt2 p329.
 2 tpis91 SN  1.00I   2.00    0.00    0.00    0.00 0  372.5189400      -8066.737
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14883.263
-5.739254890D+03-9.435024450D+01 7.377956660D+00-8.258348940D-04 1.011687040D-06
-6.508451600D-10 1.708186600D-13               -2.622644500D+03-9.605814960D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14883.263
-1.559453390D+04-1.594789414D+00 7.001351160D+00-5.935324240D-07 1.407432564D-10
-1.703457321D-14 8.233611710D-19               -3.100608319D+03 1.235038509D+00
SnI3            TPIS 1991 v2 pt1 p388; pt2 p330.
 2 tpis91 SN  1.00I   3.00    0.00    0.00    0.00 0  499.4234100      -8017.540
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20309.360
-1.069978099D+04-1.387693540D+02 1.055637633D+01-1.216435658D-03 1.490873499D-06
-9.594499630D-10 2.518810438D-13               -3.314229880D+03-1.249558209D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20309.360
-2.517534870D+04-2.348282890D+00 1.000199130D+01-8.752764840D-07 2.076464980D-10
-2.514060336D-14 1.215482266D-18               -4.017055610D+03-9.263908460D+00
SnI4            TPIS 1991 v2 pt1 p391; pt2 p332.
 2 tpis91 SN  1.00I   4.00    0.00    0.00    0.00 0  626.3278800    -118854.043
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26745.957
-1.283146793D+04-1.459885093D+02 1.358634885D+01-1.283554646D-03 1.574557147D-06
-1.013990168D-09 2.663370430D-13               -1.751178045D+04-2.367973168D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        26745.957
-2.801840706D+04-2.474699366D+00 1.300210215D+01-9.250962340D-07 2.196515817D-10
-2.661071614D-14 1.287167546D-18               -1.825083832D+04-2.027484281D+01
SnO             Hf0,Props: TPIS 1991 V2 pt1 p359; pt2 p307.
 2 tpis91 SN  1.00O   1.00    0.00    0.00    0.00 0    134.70940      21911.054
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8874.107
 2.547788022D+04-2.293583066D+02 3.421593530D+00 4.713300040D-03-7.365971320D-06
 5.379738870D-09-1.519277855D-12 0.000000000D+00 2.853047679D+03 6.673965270D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8874.107
-2.555955548D+06 7.870053500D+03-5.439768730D+00 6.307819180D-03-2.068871370D-06
 3.307074880D-10-1.848169716D-14 0.000000000D+00-4.841663910D+04 7.175952460D+01
SnO2            TPIS 1991 v2 pt1 p364; pt2 p309.
 2 tpis91 SN  1.00O   2.00    0.00    0.00    0.00 0  150.7088000      11680.180
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11795.680
 4.707674080D+04-6.114568670D+02 6.117433910D+00 7.514014660D-03-1.238371787D-05
 9.220915990D-09-2.632417597D-12                2.981068066D+03-8.144926410D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11795.680
-1.573558926D+05-1.427316788D+02 7.605700760D+00-4.198008530D-05 9.218742430D-09
-1.051372983D-12 4.849579270D-17               -5.234531870D+02-1.428360169D+01
SnS             D0,Props: TPIS 1991 V2 pt1 p394; pt2 p334.
 2 tpis91 SN  1.00S   1.00    0.00    0.00    0.00 0    150.77600     111099.012
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9301.112
 2.724877813D+04-4.924126380D+02 6.221654730D+00-3.409406960D-03 3.984913680D-06
-2.470702874D-09 6.339341460D-13 0.000000000D+00 1.452495307D+04-6.791275280D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9301.112
-1.797985129D+06 6.141736320D+03-4.019504880D+00 5.993829180D-03-2.188735204D-06
 3.899542000D-10-2.406563630D-14 0.000000000D+00-2.611349815D+04 6.256821700D+01
SnS2            TPIS 1991 v2 pt1 p365; pt2 p336.
 2 tpis91 SN  1.00S   2.00    0.00    0.00    0.00 0  182.8420000     149645.595
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13635.095
 3.877145410D+04-8.486953940D+02 1.042083990D+01-5.686902670D-03 6.373829770D-06
-3.825158100D-09 9.502480960D-13                2.006027952D+04-2.723723128D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13635.095
-6.764084050D+04-1.970189679D+01 7.515333870D+00-6.332559180D-06 1.434207625D-09
-1.676383081D-13 7.886911900D-18                1.565053629D+04-9.922728430D+00
Sn2             TPIS 1992 v2 pt1 p354; pt2 p305.
 2 tpis91 SN  2.00    0.00    0.00    0.00    0.00 0  237.4200000     421343.737
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11373.137
-1.329666654D+05 1.639179787D+03-1.902868972D+00 1.290431677D-02-1.120542242D-05
 4.502993860D-09-6.056237770D-13                4.097452710D+04 4.435408030D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11373.137
-4.275783040D+06 1.236421656D+04-8.438336170D+00 7.088056290D-03-1.712012737D-06
 1.805262952D-10-7.058656810D-15               -3.001418720D+04 1.005138538D+02
Sr              Hf:TPIS 1996. NSRDS-NBS 35 1971 p189. NSRDS-NBS 34 1970.
 3 g 1/98 SR  1.00    0.00    0.00    0.00    0.00 0   87.6200000     160500.000
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    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.190649840D+00-6.304437580D-02 2.500373027D+00-1.115455943D-06 1.785248643D-09
-1.456209589D-12 4.750132981D-16                1.855852648D+04 5.555772840D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.489414410D+07-4.375335050D+04 5.137266280D+01-2.592566025D-02 6.582990000D-06
-6.949611800D-10 2.417779662D-14                2.977545522D+05-3.454890770D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 5.562233720D+08-6.093193220D+05 2.109096848D+02-3.010063957D-02 2.178021676D-06
-7.824003460D-11 1.109909620D-15                4.579268340D+06-1.752716908D+03
Sr+             Spec:NSRDS-NBS 35 vII 1971 p191
 3 g 1/98 SR  1.00E  -1.00    0.00    0.00    0.00 0   87.6194514     716166.328
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.127287678D+01-1.346951870D-01 2.500651495D+00-1.635163061D-06 2.249493149D-09
-1.610827539D-12 4.698612333D-16                8.538981180D+04 6.247259240D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 3.145095058D+06-9.514756890D+03 1.350086948D+01-6.059717120D-03 1.594068746D-06
-1.718800946D-10 6.322256169D-15                1.457991907D+05-7.236416930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 9.016769220D+08-6.244641660D+05 1.695763594D+02-2.154835606D-02 1.462482744D-06
-4.930465390D-11 6.505705019D-16                4.966238870D+06-1.431844579D+03
SrBr            D0,TabData(extrap):TPIS 1996 pt1 p522; pt2 p402.
 3 tpis96 SR  1.00BR  1.00    0.00    0.00    0.00 0  167.5240000    -63917.691
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10107.109
-7.549771000D+02-7.359527950D+01 4.828030270D+00-7.160583510D-04 1.028527296D-06
-6.888370590D-10 1.880258006D-13               -8.686168480D+03 4.151146610D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10107.109
 3.009971950D+06-9.193179880D+03 1.526031790D+01-6.009246180D-03 1.692609691D-06
-2.039435815D-10 8.807764460D-15                4.922798280D+04-7.068244450D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10107.109
 2.274960708D+08-1.565996629D+05 4.234579280D+01-3.477056190D-03 1.358735476D-07
-2.622981311D-12 1.969250076D-17                1.221439274D+06-3.265824550D+02
SrBr2           Hsubl,cons: TPIS v3 pt1 p524; pt2 p404.
 2 tpis96 SR  1.00BR  2.00    0.00    0.00    0.00 0  247.4280000   -406725.851
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16334.649
-4.632458660D+03-7.244938640D+01 7.800217160D+00-6.772125310D-04 8.537780240D-07
-5.632351740D-10 1.510568795D-13               -5.082238330D+04-5.285074760D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16334.649
-1.186173059D+04-1.404383013D+00 7.501215570D+00-5.415983190D-07 1.296969275D-10
-1.580911652D-14 7.681582270D-19               -5.118575210D+04-3.552037110D+00
SrCL            D0,TabData(extrap):TPIS 1996 pt1 p515; pt2 p398.
 3 tpis96 SR  1.00CL  1.00    0.00    0.00    0.00 0  123.0727000   -127867.894
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9800.106
 3.555352710D+03-1.729385050D+02 5.213445560D+00-1.542911058D-03 2.025836442D-06
-1.327077494D-09 3.547178910D-13               -1.588288079D+04 4.818057780D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9800.106
 2.070218603D+06-6.199893730D+03 1.150314585D+01-3.675685270D-03 9.461731540D-07
-9.203767950D-11 2.707245531D-15                2.271473097D+04-4.561059960D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9800.106
 1.382280191D+08-9.659579830D+04 2.600430844D+01-1.405208475D-03 2.007341799D-08
 7.119352020D-13-2.001270829D-17                7.448023830D+05-1.876859871D+02
SrCL+           IP(SrCL),Cons: TPIS 1996 pt1 p516; pt2 p399.
 3 g 8/98 SR  1.00CL  1.00E  -1.00    0.00    0.00 0  123.0721514     408112.162
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9582.762
 1.689043529D+03-1.749284676D+02 5.065328640D+00-9.857327840D-04 1.071655138D-06
-5.988127130D-10 1.395650932D-13                4.861190260D+04 2.491965147D-01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9582.762
-2.132475783D+04-4.057948270D+00 4.503149390D+00 3.826202380D-05 2.676951510D-09
 5.667610500D-14 1.613288103D-18                4.769326030D+04 3.637718840D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9582.762
-1.041313813D+04-7.208302400D+00 4.501589780D+00 3.937923600D-05 2.394465390D-09
 9.062292570D-14 4.723672450D-21                4.772357520D+04 3.647371680D+00
SrCL2           Hsubl,cons: TPIS v3 pt1 p518,p520; pt2 p401.
 2 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 0  158.5254000   -484813.902
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14416.098
 1.913170011D+03-2.681156951D+02 8.081334300D+00-2.393329295D-03 2.976397494D-06
-1.943902862D-09 5.174307710D-13               -5.910111850D+04-8.457833220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14416.098
-2.592716099D+04-5.263785850D+00 7.004475240D+00-1.970397814D-06 4.679671200D-10
-5.670215880D-14 2.742892387D-18               -6.045399530D+04-2.192208452D+00
SrF             D0,TabData(extrap):TPIS 1996 pt1 p507; pt2 p394.
 3 tpis96 SR  1.00F   1.00    0.00    0.00    0.00 0  106.6184032   -303552.800
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   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9283.100
 2.725004888D+04-4.850013270D+02 6.112689500D+00-3.008464623D-03 3.368460320D-06
-1.987809619D-09 4.884152090D-13              -3.536890690D+04-6.683729220D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9283.100
 8.702318590D+05-2.589812831D+03 7.200252900D+00-1.173443636D-03 1.996159570D-07
 1.103845204D-11-2.343182952D-15              -2.133675510D+04-1.667386353D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9283.100
-3.448081820D+07 2.208050499D+04-5.125700000D+00 2.209094721D-03-1.551623731D-07
 5.125512280D-12-6.680054970D-17              -2.048587612D+05 7.995564190D+01
SrF+            IP(SrF),Cons: TPIS 1996 pt1 p511; pt2 p395.
 3 g 8/98 SR  1.00F   1.00E  -1.00    0.00    0.00 0  106.6178546     209468.312
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9106.812
 4.009624200D+04-5.944946080D+02 6.182330330D+00-2.716159750D-03 2.641369127D-06
-1.383123292D-09 3.052935853D-13              2.697149351D+04-8.313659450D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9106.812
-4.752082060D+04-2.526802345D+01 4.519295280D+00 2.556426750D-05 3.382541830D-09
-1.511394636D-13 9.537491180D-18              2.383861417D+04 1.892197325D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9106.812
-2.403608095D+03-3.242568700D+01 4.507124800D+00 3.261116540D-05 1.672393446D-09
 5.130259820D-14 2.102366585D-20              2.392692006D+04 1.974517090D+00
SrF2            Hf0 & cons: TPIS v3 pt1 p514; pt2 p397.
 2 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 0  125.6168064    -784793.795
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13269.601
 4.170759650D+04-8.500132410D+02 1.002806064D+01-6.098485190D-03 7.056261330D-06
-4.359374310D-09 1.111308310D-12              -9.217859850D+04-2.325100053D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13269.601
-6.126265430D+04-1.964060822D+01 7.015557750D+00-6.512526780D-06 1.490473613D-09
-1.756437040D-13 8.317093850D-18              -9.656701250D+04-5.402308760D+00
SrH             TPIS 1996 v3 pt1 p499; pt2 p388.
 2 tpis96 SR  1.00H   1.00    0.00    0.00    0.00 0   88.6279400     219227.105
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8723.105
-4.317796890D+04 7.676429700D+02-1.594398638D+00 1.500711077D-02-1.826296898D-05
 1.136757659D-08-2.855588359D-12 0.000000000D+00 2.179685693D+04 3.324674230D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8723.105
-2.269825428D+05 1.345209458D+03 1.152194421D+00 3.109555289D-03-1.188080968D-06
 2.073091147D-10-1.300839287D-14 0.000000000D+00 1.735547062D+04 2.112916944D+01
SrI             D0,Props(extrap):TPIS 1996 pt1 p526; pt2 p405.
 3 tpis96 SR  1.00I   1.00    0.00    0.00    0.00 0  214.5244700      -7851.676
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10283.124
-2.467498501D+03-2.535495809D+01 4.603298480D+00-1.613676212D-04 2.694294049D-07
-1.564795762D-10 3.826482280D-14 0.000000000D+00-2.175538291D+03 6.411481880D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10283.124
 2.201136857D+06-7.082230700D+03 1.332597928D+01-5.305864420D-03 1.636071150D-06
-2.205540591D-10 1.078496824D-14 0.000000000D+00 4.219077170D+04-5.530833200D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10283.124
 1.557303348D+08-1.150787674D+05 3.550520760D+01-3.375329300D-03 1.695651221D-07
-4.438653930D-12 4.852777450D-17 0.000000000D+00 8.917357880D+05-2.613917335D+02
SrI2            Hsubl,cons: TPIS v3 pt1 p528; pt2 p407.
 2 tpis96 SR  1.00I   2.00    0.00    0.00    0.00 0  341.4289400    -278218.842
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16701.658
-4.391849690D+03-3.757267350D+01 7.656993500D+00-3.561721300D-04 4.508689010D-07
-2.983230473D-10 8.018658660D-14              -3.553303460D+04-2.598281578D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16701.658
-8.090381920D+03-7.348263230D-01 7.500640060D+00-2.863515042D-07 6.876556970D-11
-8.398807360D-15 4.086968160D-19              -3.572106420D+04-1.693119087D+00
SrO             D0,Props(extrap):TPIS 1996 pt1 p495; pt2 p384.
 3 tpis96 SR  1.00O   1.00    0.00    0.00    0.00 0  103.6194000     -14207.691
   200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9040.109
 4.224891670D+04-5.913517870D+02 5.964363000D+00-2.105712736D-03 2.028373972D-06
-1.197885492D-09 3.466289920D-13 0.000000000D+00 1.018053721D+02-7.511427470D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9040.109
-5.172933050D+07 1.510821000D+05-1.614513515D+02 8.516051790D-02-2.091669402D-05
 2.452307103D-09-1.108841292D-13 0.000000000D+00-9.687829520D+05 1.197846971D+03
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9040.109
 1.988729112D+08-9.438733680D+04 2.862378041D+01-2.923338947D-03 1.808436182D-07
-5.719087480D-12 7.320935570D-17 0.000000000D+00 7.583246290D+05-2.033702568D+02
SrO+            IP(SrO),Cons: TPIS 1996 pt1 p497; pt2 p386.
 3 g 8/98 SR  1.00O   1.00E  -1.00    0.00    0.00 0  103.6188514     630053.722
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10104.122
 4.618674160D+04-4.604560920D+02 5.605360720D+00-1.511707524D-03 1.328692506D-06
-6.244610540D-10 1.274632229D-13              7.694140460D+04-3.377441410D+00
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   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10104.122
 1.035147885D+06-3.339081120D+03 8.520055290D+00-2.340803237D-03 7.338594440D-07
-1.031868417D-10 5.087079240D-15                9.540749060D+04-2.491223445D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10104.122
-6.910421610D+07 1.253686165D+04 9.522159370D+00-1.279343636D-03 8.998760920D-08
-2.931863956D-12 3.752244570D-17                -5.778506890D+04-3.231958760D+01
SrOH            Hf0 & cons: TPIS v3 pt1 p502; pt2 p390.
 2 tpis96 SR  1.00O   1.00H   1.00    0.00    0.00 0  104.6273400    -194085.726
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11046.666
 4.640006560D+04-9.938685540D+02 9.784948960D+00-5.774377620D-03 5.126164110D-06
-1.833418356D-09 1.926013410D-13                -2.022721196D+04-2.740670981D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11046.666
 2.545648379D+06-7.416195980D+03 1.381956204D+01-3.096481934D-03 7.723894210D-07
-7.921280320D-11 2.740829111D-15                2.231302058D+04-6.148781130D+01
SrOH+           Hf0 & cons: TPIS v3 pt1 p503; pt2 p391.
 2 tpis96 SR  1.00O   1.00H   1.00E  -1.00    0.00 0  104.6267914     310169.605
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11104.569
 3.857366940D+04-9.030242330D+02 9.451103250D+00-5.042516280D-03 4.190101890D-06
-1.196920603D-09 1.606318743D-14                3.995067720D+04-2.601486110D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11104.569
 8.679695660D+05-2.340609538D+03 7.976829750D+00 1.023752569D-04-6.286032330D-08
 1.024851502D-11-5.723683920D-16                5.073157720D+04-2.027046917D+01
Sr(OH)2         Hf0 & cons: TPIS v3 pt1 p506; pt2 p393.
 2 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 0  121.6346800    -596694.573
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17011.921
 7.205090300D+04-1.789465226D+03 1.729429139D+01-1.169280781D-02 1.106702894D-05
-4.490146090D-09 6.603997460D-13                -6.605394040D+04-6.388681220D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17011.921
 1.750013518D+06-4.681601500D+03 1.395548402D+01 2.035019560D-04-1.253496115D-07
 2.044549432D-11-1.142004855D-15                -4.427170240D+04-5.051456850D+01
SrS             D0,Props:TPIS 1996 pt1 p529; pt2 p409.
 2 tpis96 SR  1.00S   1.00    0.00    0.00    0.00 0  119.6860000     104351.315
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9536.115
 1.256440807D+04-3.150436559D+02 5.721722510D+00-2.630479718D-03 3.384699750D-06
-2.296256846D-09 6.512086680D-13                1.277295160D+04-3.693862410D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9536.115
-1.379432947D+07 3.921331580D+04-3.602866380D+01 1.818513386D-02-3.275858160D-06
 2.324312746D-10-3.614555700D-15                -2.410246179D+05 2.991679767D+02
Sr2             D0,tabdata:Gurvich TPIS 1996 pt1 p491; pt2 p382.
 2 tpis96 SR  2.00    0.00    0.00    0.00    0.00 0  175.2400000     307570.337
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11365.137
-1.108859753D+05 5.927604010D+02 8.439688550D+00-2.652801112D-02 4.435825970D-05
-3.399915490D-08 9.965546680D-12                3.157615033D+04-7.033966650D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11365.137
 2.098445682D+05 1.038650130D+02 2.309332330D+00 1.330517507D-04-4.426433390D-08
 6.711419150D-12-3.374128000D-16                3.636642690D+04 2.168088517D+01
Ta              Hf0:TPIS vIV 1982. NSRDS-NBS 35 vIII 1971 pp149-54.
 3 g 7/97 TA  1.00    0.00    0.00    0.00    0.00 0  180.9479000     782518.638
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6199.638
-1.150907339D+04 4.780730430D+01 3.185588390D+00-5.366528160D-03 1.288379705D-05
-1.045798666D-08 3.050617695D-12                9.299797630D+04 5.336056610D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6199.638
 1.689726898D+06-5.986854660D+03 9.565039670D+00-2.511649459D-03 6.443031170D-07
-7.189237250D-11 3.113352070D-15                1.306710983D+05-4.335096270D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6199.638
-8.413419560D+08 6.381509040D+05-1.856031850D+02 2.797353600D-02-2.073321805D-06
 7.397299170D-11-1.017863944D-15                -4.836410620D+06 1.607007750D+03
Ta+             NSRDS NBS 35 vIII 1971 pp149-55.
 3 g 7/97 TA  1.00E  -1.00    0.00    0.00    0.00 0  180.9473514    1549679.335
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6337.835
 2.869712865D+05-3.084920994D+03 1.430679704D+01-1.984772164D-02 1.951445133D-05
-8.970946030D-09 1.501974665D-12                2.013828712D+05-6.306427830D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6337.835
 3.656142130D+06-1.254073524D+04 1.865022579D+01-7.943274660D-03 2.151786937D-06
-2.816764844D-10 1.413722944D-14                2.636876455D+05-1.065864286D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6337.835
 3.724273560D+07-3.405709310D+04 1.630056321D+01-2.064987830D-03 1.616826024D-07
-5.752060330D-12 7.636581870D-17                4.405115500D+05-1.040237652D+02
Ta-             JPCRD v14 n3 1985 p731.
 3 g 9/97 TA  1.00E   1.00    0.00    0.00    0.00 0  180.9484486     745469.429
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6416.129
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 1.873982301D+05-1.681268679D+03 6.480040150D+00-2.254355782D-04 2.028434876D-06
-4.679801430D-09 1.997027996D-12              9.793496020D+04-2.049618155D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6416.129
-4.235467480D+06 1.101056361D+04-4.736911070D+00 2.503562129D-03-4.821851690D-07
 4.886408030D-11-2.030547835D-15              1.574699408D+04 6.491802700D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6416.129
 4.149884030D+05 1.227972146D+03 2.209211582D+00 3.401090760D-05-2.136872502D-09
 6.906775410D-14-9.017779200D-19              8.249065600D+04 1.195636187D+01
TaCL5           JANAF data.
 2 j12/74 TA  1.00CL  5.00    0.00    0.00    0.00 0  358.2114000    -764835.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26869.100
 6.306483290D+04-1.771221442D+03 2.255083356D+01-1.360238041D-02 1.613009806D-05
-1.016307761D-08 2.631917453D-12             -8.792737110D+04-8.097864910D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       26869.100
-1.426444545D+05-3.894340320D+01 1.603142370D+01-1.333676355D-05 3.084307611D-09
-3.663930060D-13 1.745841795D-17             -9.701297170D+04-4.256987000D+01
TaO
 2 J12/73 TA  1.00O   1.00    0.00    0.00    0.00 0  196.9473000     192468.826
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.934010800D+00 3.059203800D-03-1.939636400D-06
 1.628883000D-10 3.015253500D-13              2.215447200D+04 1.145464600D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.499660300D+00 1.511253500D-03-6.538457800D-07
 1.778431400D-10-1.691940500D-14              2.199415100D+04 8.526958990D+00
TaO2
 2 J12/73 TA  1.00O   2.00    0.00    0.00    0.00 0  212.9467000    -200835.093
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.180382600D+00 9.470280500D-03-8.734686800D-06
 2.452268900D-09 3.365342100D-13             -2.545176200D+04 1.313035300D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.970166900D+00 1.179212800D-03-5.651741300D-07
 1.311378700D-10-1.056443700D-14             -2.616948100D+04-1.073998010D+00
Ti              Hf:CODATA 1989. JPCRD v14 sup2 1985.
 3 g 7/97 TI  1.00    0.00    0.00    0.00    0.00 0   47.8670000     473000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7539.141
-4.570179400D+04 6.608092020D+02 4.295257490D-01 3.615029910D-03-3.549792810D-06
 1.759952494D-09-3.052720871D-13              5.270947930D+04 2.026149738D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7539.141
-1.704786714D+05 1.073852803D+03 1.181955014D+00 2.245246352D-04 3.091697848D-07
-5.740027280D-11 2.927371014D-15              4.978069910D+04 1.740431368D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7539.141
 1.152797766D+09-7.222408380D+05 1.777167465D+02-2.008059096D-02 1.221052354D-06
-3.811452080D-11 4.798092423D-16              5.772614540D+06-1.518080466D+03
Ti+             JPCRD v14 sup2 1985.
 3 g 7/97 TI  1.00E  -1.00    0.00    0.00    0.00 0   47.8664514    1137624.029
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7899.829
 1.707457044D+05-1.727524602D+03 9.615885330D+00-1.089655060D-02 8.201809650D-06
-2.871464413D-09 3.420382976D-13              1.447897558D+05-3.463143660D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7899.829
-7.685463080D+05 2.545868100D+03 3.423862780D-01 7.099901360D-04 2.706231875D-08
-2.371660100D-11 1.895443077D-15              1.198821489D+05 2.484799150D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7899.829
 3.918035620D+07-2.534581605D+04 9.586759720D+00-7.584155410D-04 4.432999350D-08
-8.442571760D-13-4.517128089D-19              3.344440620D+05-5.220026270D+01
Ti-             JPCRD v14 n3 1985 p731.
 3 g 9/97 TI  1.00E   1.00    0.00    0.00    0.00 0   47.8675486     459203.814
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7562.614
-3.006484990D+03 2.040911689D+02 1.822638976D+00 1.245254812D-03-1.309239865D-06
 7.372143220D-10-1.724319779D-13              5.346772050D+04 1.205926588D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7562.614
 2.341117640D+04 2.580413872D+00 2.497754577D+00 9.769072040D-07-2.280024955D-10
 2.717202291D-14-1.295670294D-18              5.454662180D+04 7.999823950D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7562.614
 1.417514172D+04 5.638799640D+00 2.498751709D+00 1.426579908D-07-8.889194940D-12
 2.867172222D-16-3.746329300D-21              5.451843520D+04 7.994109450D+00
TiCL
 2 J12/68 TI  1.00CL  1.00    0.00    0.00    0.00 0   83.3197000     154393.163
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.854308900D+00 7.959334500D-03-9.821116200D-06
 5.241998100D-09-9.798617700D-13              1.744121600D+04 1.172999060D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 5.296976000D+00-1.640169200D-04 1.571976100D-07
-3.856708900D-11 3.073966300D-15                1.685767400D+04-4.947066910D-01
TiCL2
 2 J12/68 TI  1.00CL  2.00    0.00    0.00    0.00 0  118.7724000    -237237.623
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.972347500D+00 1.127733500D-02-2.058191600D-05
 1.718665000D-08-5.404959000D-12                -3.036628500D+04 2.558932210D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.762485200D+00-9.387242500D-04 8.012151800D-07
-1.904803000D-10 1.496154500D-14                -3.091580500D+04-1.075276530D+01
TiCL3
 2 J12/68 TI  1.00CL  3.00    0.00    0.00    0.00 0  154.2251000    -539328.974
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.880155700D+00 3.355893300D-02-5.995746000D-05
 4.886366400D-08-1.509099200D-11                -6.677602300D+04 1.395808240D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.000810300D+01 4.193637400D-04-2.150487300D-07
 4.533701800D-11-3.454683800D-15                -6.806125000D+04-1.951077960D+01
TiCL4
 2 J12/67 TI  1.00CL  4.00    0.00    0.00    0.00 0  189.6778000    -763178.781
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.949675700D+00 2.604965900D-02-4.652030200D-05
 3.838483400D-08-1.202791500D-11                -9.467783100D+04-2.925853740D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.238603000D+01 7.093131600D-04-3.174607800D-07
 6.260395800D-11-4.533703800D-15                -9.566907800D+04-2.847169840D+01
TiO
 2 J12/73 TI  1.00O   1.00    0.00    0.00    0.00 0   63.8664000      54392.051
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.119888100D+00 3.120248700D-03-1.329707300D-06
-1.333836200D-09 9.631582800D-13                5.486871900D+03 9.442306740D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.136017600D+00 7.392645800D-04-4.544446400D-07
 1.304365800D-10-1.152255700D-14                5.198348300D+03 4.122065140D+00
TiOCL
 2 J 9/63 TI  1.00O   1.00CL  1.00    0.00    0.00 0   99.3191000    -244267.698
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.409385600D+00 1.517055400D-02-2.442848300D-05
 1.873452100D-08-5.568068400D-12                -3.088784600D+04 8.694229850D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.831992400D+00 7.635938700D-04-3.395308900D-07
 6.666706900D-11-4.813294600D-15                -3.158231100D+04-7.754012450D+00
TiOCL2
 2 J 9/63 TI  1.00O   1.00CL  2.00    0.00    0.00 0  134.7718000    -545564.732
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.440814000D+00 1.770504900D-02-2.952524100D-05
 2.324732800D-08-7.047977700D-12                -6.780685400D+04 3.450628570D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.336865500D+00 7.596998700D-04-3.382737800D-07
 6.648386300D-11-4.803379300D-15                -6.857264500D+04-1.514432190D+01
TiO2
 2 J12/73 TI  1.00O   2.00    0.00    0.00    0.00 0   79.8658000    -305440.771
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.014271700D+00 1.094210100D-02-1.287858800D-05
 7.118952900D-09-1.492751000D-12                -3.802050100D+04 1.136415340D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.845506100D+00 1.393821300D-03-6.640306200D-07
 1.385738000D-10-9.884218400D-15                -3.870059300D+04-2.796243170D+00
V              Hf0:TPIS v4 1982 p60.  Levels:JPCRD v14 sup2 1985.
 3 g 7/97 V   1.00    0.00    0.00    0.00    0.00 0   50.9415000     517267.064
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7907.064
-5.535376020D+04 5.593338510D+02 2.675543482D+00-6.243049630D-03 1.565902337D-05
-1.372845314D-08 4.168388810D-12                5.820664360D+04 9.524567490D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7907.064
 1.200390300D+06-5.027005300D+03 1.058830594D+01-5.044326100D-03 1.488547375D-06
-1.785922508D-10 8.113013866D-15                9.170740910D+04-4.768336320D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7907.064
 2.456040166D+09-1.339992028D+06 2.781039851D+02-2.638937359D-02 1.303527149D-06
-3.214680330D-11 3.099999094D-16                1.087152043D+07-2.439954380D+03
V+             Levels:JPCRD v14 sup2 1985.
 3 g 7/97 V   1.00E  -1.00    0.00    0.00    0.00 0   50.9409514    1173745.411
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    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7897.811
 7.568834460D+04-8.415273820D+02 7.559232710D+00-1.441722656D-02 2.038356397D-05
-1.289073883D-08 3.065656561D-12                1.444478191D+05-1.991067645D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7897.811
 2.347072054D+06-9.021197190D+03 1.477349798D+01-6.891896880D-03 1.968884877D-06
-2.539798544D-10 1.226783122D-14                1.958351444D+05-7.855592930D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7897.811
 2.516527258D+08-1.866476656D+05 5.633587110D+01-7.198536950D-03 5.074401490D-07
-1.699749225D-11 2.157800037D-16                1.585980536D+06-4.512822600D+02
V-             JPCRD v14 n3 1985 p731.
 3 g 9/97 V   1.00E   1.00    0.00    0.00    0.00 0   50.9420486     460386.063
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7878.263
-3.799273560D+03 2.313840448D+02 1.725608190D+00 1.429275357D-03-1.506038188D-06
 8.491815170D-10-1.987980413D-13                5.347402920D+04 1.261900982D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7878.263
 2.600100430D+04 2.096334097D+00 2.498006548D+00 8.991278840D-07-2.139749508D-10
 2.581021334D-14-1.240812796D-18                5.470007080D+04 7.977900240D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7878.263
 1.601102910D+04 5.820974900D+00 2.498705489D+00 1.484212570D-07-9.272956840D-12
 2.997799727D-16-3.924862230D-21                5.466692550D+04 7.974557420D+00
VCL4
 2 G 2/76 V   1.00CL  4.00    0.00    0.00    0.00 0  192.7523000    -525521.534
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.116646200D+00 2.542321700D-02-4.549901700D-05
 3.758388600D-08-1.178034400D-11               -6.612389300D+04-2.330954750D+00
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.271864700D+01 1.660017600D-05 1.416149800D-07
-3.476183300D-11 2.288976300D-15               -6.718799200D+04-2.884801030D+01
VN
 2 J12/73 V   1.00N   1.00    0.00    0.00    0.00 0   64.9482400     523013.121
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.723359000D+00 4.164298900D-03-2.191281200D-06
-1.235187200D-09 1.079183300D-12                6.192789300D+04 1.141735790D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.185228000D+00 6.151472000D-04-3.577633500D-07
 1.074886200D-10-9.727550500D-15                6.151154000D+04 3.776186610D+00
VO
 2 J12/73 V   1.00O   1.00    0.00    0.00    0.00 0   66.9409000     127615.031
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.943844100D+00 2.905923400D-03-9.951657500D-07
-1.408659200D-09 9.243850800D-13                1.435274600D+04 1.018643100D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.911470200D+00 7.754779200D-04-4.226378600D-07
 1.160883800D-10-1.007072400D-14                1.406520400D+04 5.071854090D+00
VO2
 2 J12/73 V   1.00O   2.00    0.00    0.00    0.00 0   82.9403000    -232634.437
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.193785900D+00 9.297945700D-03-8.342246900D-06
 2.104917000D-09 4.458264500D-13               -2.927549100D+04 1.128721900D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.947014700D+00 1.168677900D-03-5.053637900D-07
 9.672361100D-11-6.824588300D-15               -2.998380200D+04-2.738025110D+00
W              Hf0:TPIS v4 1982. NSRDS-NBS 35 v3 1971;NSRDS-NBS 34 1970
 3 g 4/98 W   1.00    0.00    0.00    0.00    0.00 0  183.8400000     851243.526
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6216.526
 1.595223922D+05-2.673843928D+03 2.060469727D+01-6.252315230D-02 1.105654838D-04
-8.453511610D-08 2.336187771D-11                1.139648616D+05-9.011836900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6216.526
-8.048745960D+06 1.465700424D+04-2.508531501D-01-2.596486992D-03 1.409225475D-06
-2.233011706D-10 1.262640862D-14               -3.091130919D+03 3.955822190D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6216.526
 1.421636486D+09-4.325365550D+05-8.841615070D+00 1.645538940D-02-1.908373835D-06
 8.530482890D-11-1.360501851D-15                3.994798750D+06-1.266418236D+01
W+             NSRDS,NBS 35 vIII 1971 p162
 3 g 7/97 W   1.00E  -1.00    0.00    0.00    0.00 0  183.8394514    1627840.965
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6221.265
-1.969284929D+05 2.670137332D+03-1.131686913D+01 3.308183730D-02-3.629035500D-05
 2.066142971D-08-4.808285562D-12                1.820950862D+05 8.552104480D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6221.265
 6.387743400D+06-2.061811463D+04 2.759291576D+01-1.244535845D-02 3.271200490D-06
-4.065463720D-10 1.912595872D-14                3.245174430D+05-1.716919194D+02
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   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6221.265
 6.839559150D+07-8.981711810D+04 3.845720800D+01-5.465752290D-03 4.024981150D-07
-1.342970538D-11 1.667637540D-16              8.546932820D+05-2.892805521D+02
W-            JPCRD v14 n3 1985 p731.
 3 g 1/99 W   1.00E   1.00    0.00    0.00    0.00 0  183.8405486     766391.528
   298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              9.142981370D+04 8.461169670D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              9.142981370D+04 8.461169670D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              9.142981370D+04 8.461169670D+00
WCL6          JANAF 12/66. JPCRD v14 sup1 1985.
 2 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 0  396.5562000    -493712.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30790.955
 3.339391670D+04-1.697366080D+03 2.560612352D+01-1.425247881D-02 1.739682668D-05
-1.120537864D-08 2.951522890D-12             -5.673059240D+04-9.741466980D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30790.955
-1.516735473D+05-3.451379250D+01 1.902867176D+01-1.242486969D-05 2.917675103D-09
-3.505981440D-13 1.685355887D-17             -6.535779790D+04-5.894915640D+01
WOCL4         JANAF 6/67. JPCRD v14 sup1 1985.
 2 j 6/67 W   1.00O   1.00CL  4.00    0.00    0.00 0  341.6502000    -573493.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22271.379
 2.658812693D+04-9.336913240D+02 1.321377385D+01 1.270930811D-02-1.964716509D-05
 1.405106974D-08-3.899382140D-12             -6.792290790D+04-3.594870210D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22271.379
-3.049028285D+05-3.539425860D+02 1.626432703D+01-1.058245461D-04 2.340548846D-08
-2.685852021D-12 1.245412684D-16             -7.272546740D+04-4.991761780D+01
WO2           TPIS 1982 pt1 p47 pt2 p50.
 2 tpis82 W   1.00O   2.00    0.00    0.00    0.00 0  215.8388000      29061.744
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10714.848
 3.120918919D+03 2.413883468D+02-3.024119184D-01 2.324333417D-02-3.378812680D-05
 2.380934019D-08-6.421592880D-12              1.442005265D+03 2.957655179D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10714.848
-7.537406680D+05 3.204643050D+03 6.701965600D-01 4.488238870D-03-8.858328460D-07
 6.245171750D-11-9.046613900D-16             -1.769420230D+04 3.405724010D+01
WO2CL2        JANAF 6/73. JPCRD v14 sup1 1985.
 2 j 6/73 W   1.00O   2.00CL  2.00    0.00    0.00 0  286.7442000    -671532.000
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19503.817
 4.300154480D+02-2.438547856D+02 7.976306990D+00 1.715005722D-02-2.487975176D-05
 1.737644163D-08-4.771928400D-12             -8.232812400D+04-7.844774560D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19503.817
-2.404791730D+05-3.068379644D+02 1.322814502D+01-9.100220710D-05 2.006581020D-08
-2.296837607D-12 1.062829386D-16             -8.367493060D+04-3.491556940D+01
WO3           TPIS 1982 pt1 p50 pt2 p52.
 2 tpis82 W   1.00O   3.00    0.00    0.00    0.00 0  231.8382000    -319725.213
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13267.943
 7.262461460D+03 3.429391090D+01 1.573061955D+00 2.754971099D-02-3.994827310D-05
 2.809371537D-08-7.777545730D-12             -4.001733270D+04 1.857409963D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13267.943
 1.732203640D+06-6.284719780D+03 1.681358864D+01-3.472089360D-03 8.079935800D-07
-6.589378720D-11 1.142928957D-15             -2.473075565D+03-7.407474090D+01
WO3-          TPIS 1982 pt1 p51 pt2 p53.
 2 tpis82 W   1.00O   3.00E   1.00    0.00    0.00 0  231.8387486    -650475.961
   298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13714.639
 1.630999684D+05-1.967609682D+03 1.201970914D+01 1.681260779D-03-5.859360060D-06
 5.028616330D-09-1.434012198D-12 0.000000000D+00-7.009203990D+04-3.936901040D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13714.639
 4.637832510D+05-1.347089334D+03 9.773637560D+00 1.071395459D-03-3.842403660D-07
 5.737531900D-11-3.157605982D-15 0.000000000D+00-7.239515570D+04-2.391116343D+01
(WO3)2        TPIS 1982 pt1 p52 pt2 p54.
 2 tpis82 W   2.00O   6.00    0.00    0.00    0.00 0  463.6764000   -1210443.298
   200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       25543.014
 8.088414510D+04-9.060340790D+02 7.601575390D+00 5.241008510D-02-7.922356390D-05
 5.708640180D-08-1.606775042D-11             -1.441496996D+05-1.093524051D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       25543.014
-6.674072430D+05-7.032518360D+02 2.251617461D+01-2.035473339D-04 4.444320340D-08
-5.045188080D-12 2.318375739D-16             -1.502699479D+05-8.613988980D+01
(WO3)3        TPIS 1982 pt1 p53 pt2 p55.
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 2 tpis82 W   3.00O   9.00    0.00    0.00    0.00 0  695.5146000   -2013291.101
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       40688.367
 3.485390010D+04-1.933496319D+02 8.206544780D+00 8.599515510D-02-1.257565252D-04
 8.891567220D-08-2.471213564D-11              -2.462453469D+05-5.657325260D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       40688.367
-9.450263310D+05-1.133837222D+03 3.483479230D+01-3.301361100D-04 7.226602130D-08
-8.221581630D-12 3.785050840D-16              -2.488486308D+05-1.441551053D+02
(WO3)4          TPIS 1982 pt1 p54 pt2 p56.
 2 tpis82 W   4.00O  12.00    0.00    0.00    0.00 0  927.3528000   -2817433.885
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       54538.739
 1.388606167D+04 2.287518563D+02 8.662370000D+00 1.219700696D-01-1.770499494D-04
 1.246790033D-07-3.456182860D-11              -3.467839600D+05-3.603937290D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       54538.739
-1.277530217D+06-1.566538532D+03 4.715363520D+01-4.563263220D-04 9.990758360D-08
-1.136816181D-11 5.234399340D-16              -3.477418470D+05-2.051588395D+02
(WO3)5          TPIS 1982 pt1 p56 pt2 p57.
 2 tpis82 W   5.00O  15.00    0.00    0.00    0.00 0 1159.1910000   -3551492.326
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       68473.453
 1.497576743D+04 2.719999782D+02 1.138626896D+01 1.523302100D-01-2.211447753D-04
 1.557377753D-07-4.317244680D-11              -4.371424320D+05-1.441643481D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       68473.453
-1.600667953D+06-1.958437864D+03 5.944227390D+01-5.705105630D-04 1.249090916D-07
-1.421320416D-11 6.544458260D-16              -4.384095860D+05-2.660238838D+02
Xe              Ref-Elm. Spec: NSRDS-NBS 35 1971; NSRDS-NBS 34 1970.
 3 g 1/99 XE  1.00    0.00    0.00    0.00    0.00 0  131.2900000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.453750000D+02 6.164419930D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.025226680D+03-1.209507521D+01 2.514153347D+00-8.248102080D-06 2.530232618D-09
-3.892333230D-13 2.360439138D-17              -6.685800730D+02 6.063676440D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 2.540397456D+08-1.105373774D+05 1.382644099D+01 1.500614606D-03-3.935359030D-07
 2.765790584D-11-5.943990574D-16               9.285443830D+05-1.109834899D+02
Xe+             Moore: NSRDS-NBS 35 1971; NSRDS-NBS 34 1970.
 3 g 3/97 XE  1.00E  -1.00    0.00    0.00    0.00 0  131.2894514    1176552.232
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 1.002923620D+02-1.218753648D+00 2.506016493D+00-1.547411334D-05 2.191372741D-08
-1.623684074D-11 4.929132670D-15               1.407665368D+05 7.516678190D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.241683887D+04-1.500654643D+02 2.964678293D+00-4.693396660D-04 1.959138719D-07
-3.037761925D-11 1.637361082D-15               1.414966808D+05 4.565651460D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.562275878D+08 1.570476914D+05-3.635537230D+01 5.019392580D-03-3.438107240D-07
 1.140544651D-11-1.295661530D-16              -1.103556546D+06 3.436188470D+02
Zn              Hf:CODATA 1989. JPCRD v24 n6 1995 p1803.
 3 g 6/97 ZN  1.00    0.00    0.00    0.00    0.00 0   65.3900000     130400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.493805072D+04 5.118861010D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-1.755591489D+05 4.984139240D+02 1.969386292D+00 2.608808787D-04-5.627195080D-08
 2.723336049D-12 4.266685808D-16               1.173773458D+04 8.961085650D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-2.087287962D+08 1.578178131D+05-3.622033110D+01 3.345230020D-03-8.567422720D-09
-7.122544740D-12 1.691187274D-16              -1.217847671D+06 3.459439960D+02
Zn+             JPCRD v24 n6 1995 pp1803-72.
 3 g 6/97 ZN  1.00E  -1.00    0.00    0.00    0.00 0   65.3894514    1043000.128
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21               1.246979918D+05 5.811995500D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-3.436179460D+05 9.567355240D+02 1.511478952D+00 4.613467960D-04-8.786800980D-08
 7.558567780D-13 1.168827311D-15               1.185321933D+05 1.300742670D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6197.428
-3.011747676D+09 2.074729347D+06-5.589526960D+02 7.501396440D-02-5.136763100D-06
 1.741662147D-10-2.323920111D-15              -1.609057856D+07 4.824788010D+03
Zr              Hf:TPIS 1982. Spec:NSRDS-NBS 35 v2 1971;JCP v85 n6 1986.
 3 g 1/98 ZR  1.00    0.00    0.00    0.00    0.00 0   91.2240000     599318.611
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6815.611
 6.715899960D+04-9.435981740D+02 6.359756180D+00-9.790119730D-04-7.608224150D-06
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 9.308717430D-09-3.124675586D-12                7.588019470D+04-1.665770522D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6815.611
 6.006771840D+06-1.566960605D+04 1.796982350D+01-6.763409650D-03 1.733678968D-06
-2.064699786D-10 9.334092610D-15                1.734636249D+05-1.051117377D+02
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6815.611
 5.207701380D+08-2.825652444D+05 6.077054350D+01-5.081211410D-03 2.345845819D-07
-6.237212120D-12 8.010718759D-17                2.351487351D+06-5.093183060D+02
Zr+             Spec:NSRDS-NBS 35 vII 1971. IP:NSRDS-NBS v34 1970.
 3 g 1/98 ZR  1.00E  -1.00    0.00    0.00    0.00 0   91.2234514    1246246.292
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7471.892
 1.739842193D+05-2.224598466D+03 1.400787829D+01-2.378785396D-02 2.641058912D-05
-1.442565487D-08 3.135982142D-12                1.598210714D+05-5.816728810D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7471.892
 7.298137160D+05-2.017117556D+03 5.037498300D+00-5.503371950D-04 1.023753499D-07
-1.261537793D-11 7.092401042D-16                1.620884945D+05-9.820640860D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7471.892
-2.294818875D+07 1.860972745D+04-1.661509984D+00 6.020341290D-04-3.930742580D-08
 1.543806931D-12-2.618341088D-17                4.907298890D+03 4.642130480D+01
Zr-             JPCRD v14 n3 1985 p731.
 3 g 2/98 ZR  1.00E   1.00    0.00    0.00    0.00 0   91.2245486     552952.398
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7749.498
 3.046662367D+04-8.074277210D+02 9.213006110D+00-1.614342054D-02 1.908653551D-05
-1.138888914D-08 2.745019116D-12                6.903034030D+04-2.862644371D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7749.498
 8.471861160D+04 3.175439340D+02 2.251491246D+00 1.018645389D-04-2.285208242D-08
 2.647293502D-12-1.235813604D-16                6.422337600D+04 1.081261057D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7749.498
-4.386641560D+05 3.768748730D+02 2.417088403D+00 9.411538660D-06-5.824251210D-10
 1.866281342D-14-2.423724320D-19                6.334701050D+04 9.677778690D+00
ZrN
 2 J 6/63 ZR  1.00N   1.00    0.00    0.00    0.00 0  105.2307400     713372.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.071887170D+00 2.643004740D-03 3.184994280D-07
-3.633505810D-09 2.026795640D-12                8.476849470D+04 9.805889870D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.143789220D+00 4.043072130D-04-1.446331070D-07
 2.476063740D-11-1.542802020D-15                8.446142000D+04 4.159379060D+00
ZrO             TPIS 1982 v4 pt1 p118; pt2 p118.
 3 tpis82 ZR  1.00O   1.00    0.00    0.00    0.00 0  107.2234000      83922.708
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8970.108
-5.091761400D+05 8.652770090D+03-5.294740150D+01 1.728961761D-01-2.457230895D-04
 1.672135156D-07-4.423012380D-11 0.000000000D+00-3.095129818D+04 3.132576719D+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8970.108
 4.648098310D+05 3.442314470D+02 4.815779180D+00-4.660633140D-04 2.140489079D-07
-2.054364483D-11 4.084667760D-16 0.000000000D+00 7.317340700D+03 1.502933548D+00
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8970.108
 1.343456923D+08-7.851088360D+04 1.981614195D+01-8.027211020D-04 2.522081797D-09
 7.959625600D-13-1.684162816D-17 0.000000000D+00 6.406670590D+05-1.358472283D+02
ZrO+            TPIS 1982 v4 pt1 p122; pt2 p120.
 3 tpis82 ZR  1.00O   1.00E  -1.00    0.00    0.00 0  107.2228514     720614.114
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9464.114
 1.032911549D+04 7.304661220D+01 2.606345299D+00 5.099300290D-03-6.250338760D-06
 3.797460020D-09-9.198416900D-13 0.000000000D+00 8.533233780D+04 1.267311019D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9464.114
-4.937166560D+05 6.699900760D+02 4.575353470D+00-6.923237900D-04 4.280600940D-07
-7.547660220D-11 4.414279860D-15 0.000000000D+00 8.018880660D+04 2.928943704D+00
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9464.114
 4.389941590D+07-2.084044161D+04 8.167126240D+00-5.668596640D-05-8.861355220D-09
 4.773106180D-13-7.435660480D-18 0.000000000D+00 2.554517908D+05-3.127152387D+01
ZrO2
 2 J12/65 ZR  1.00O   2.00    0.00    0.00    0.00 0  123.2228000    -286189.801
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.210377900D+00 1.162897600D-02-1.557536000D-05
 1.004424300D-08-2.543889000D-12               -3.577561200D+04 1.177386770D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.141854500D+00 9.770369500D-04-4.333718200D-07
 8.495458900D-11-6.126664800D-15               -3.644617800D+04-2.709789120D+00
Ag(cr)          Silver Cubic Crystal. CODATA,1989, p228.
 1 coda89 AG  1.00    0.00    0.00    0.00    0.00 0  107.8682000          0.000
    200.000   1235.0807 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5745.000
-7.099236470D+04 7.254788020D+02 1.066518380D-01 5.529541550D-03-4.425590850D-06
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 2.091668120D-09-3.888924460D-13              -4.614014260D+03 5.074216040D+00
Ag(L)          Silver Liquid. CODATA,1989, p228.
 1 coda89 AG  1.00    0.00    0.00    0.00    0.00 2  107.8682000         0.000
   1235.080   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5745.000
 0.000000000D+00 0.000000000D+00 4.017073770D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.672269970D+02-1.771527070D+01
AL(cr)         Aluminum Cubic Crystal. CODATA 1989, p217.
 1 coda89 AL  1.00    0.00    0.00    0.00    0.00 1   26.9815380         0.000
    200.000    933.6107 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4540.000
-6.251811430D+04 6.343934350D+02-7.131883820D-01 1.088725280D-02-1.458741820D-05
 9.961160880D-09-1.774928010D-12              -3.985439320D+03 6.561100200D+00
AL(L)          Aluminum Liquid. CODATA 1989, p217.
 1 coda89 AL  1.00    0.00    0.00    0.00    0.00 2   26.9815380         0.000
    933.610   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4540.000
 0.000000000D+00 0.000000000D+00 3.818625510D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.576323160D+01-1.752553420D+01
ALBr3(cr)       Monoclinic. Gurvich TPIS 1996 pt1 p187,115 pt2 p150.
 1 tpis96 AL  1.00BR  3.00    0.00    0.00    0.00 1  266.6935380    -511500.000
    200.000    371.1607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21920.000
-1.907292099D+05 0.000000000D+00 2.665662652D+01-8.326099820D-02 1.395828123D-04
 0.000000000D+00 0.000000000D+00              -6.763881140D+04-1.126522667D+02
ALBr3(L)        Liquid. Gurvich TPIS 1996 pt1 p187,115 pt2 p150.
 1 tpis96 AL  1.00BR  3.00    0.00    0.00    0.00 2  266.6935380    -511500.000
    371.160   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21920.000
 0.000000000D+00 0.000000000D+00 1.503395871D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.481402080D+04-6.083617689D+01
ALCL3(cr)       Monoclinic. Gurvich TPIS 1996 pt1 p172-3,115 pt2 p133.
 1 tpis96 AL  1.00CL  3.00    0.00    0.00    0.00 1  133.3396380    -705100.000
    200.000    465.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16980.000
-2.605551108D+05 2.535762396D+03-1.248379067D+00 2.465425813D-02-8.048550150D-06
 0.000000000D+00 0.000000000D+00              -1.007777032D+05 2.030375677D+01
ALCL3(L)        Liquid. Gurvich TPIS 1996 pt1 p172-3,115 pt2 p133.
 1 tpis96 AL  1.00CL  3.00    0.00    0.00    0.00 2  133.3396380    -705100.000
    465.700   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16980.000
 0.000000000D+00 0.000000000D+00 1.509409454D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.559022460D+04-6.519014639D+01
ALF3(II)        Hexagonal. Gurvich TPIS 1996 pt1 p156,115 pt2 p119.
 2 tpis96 AL  1.00F   3.00    0.00    0.00    0.00 1   83.9767476   -1510400.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11620.400
 0.000000000D+00 0.000000000D+00-2.444621150D+00 6.248607440D-02-8.043962500D-05
 0.000000000D+00 0.000000000D+00              -1.829961207D+05 6.871585170D+00
    298.150   1273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11620.400
 0.000000000D+00 0.000000000D+00-3.158574588D+00 7.101368571D-02-1.246540085D-04
 7.930377136D-08 0.000000000D+00              -1.829283321D+05 9.661469435D+00
ALF3(I)         Cubic. Gurvich TPIS 1996 pt1 p156,115 pt2 p119.
 1 tpis96 AL  1.00F   3.00    0.00    0.00    0.00 2   83.9767476   -1510400.000
    728.000   2100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11620.400
-1.060675855D+05 0.000000000D+00 1.114052422D+01 1.092668119D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.853502219D+05-5.651122021D+01
ALH3(a)         Alpha,hexagonal. TPIS 1996 pt1 pp144-5, pt2 p108.
 1 tpis96 AL  1.00H   3.00    0.00    0.00    0.00 1   30.0053580    -11400.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5440.000
 5.744612990D+05-7.649579650D+03 3.481355430D+01-4.495737990D-02 2.948551342D-05
 0.000000000D+00 0.000000000D+00               3.549793150D+04-2.050727589D+02
ALI3(cr)        Hexagonal. TPIS 1996 pt1 p193-5,115 pt2 p155.
 1 tpis96 AL  1.00I   3.00    0.00    0.00    0.00 1  407.6949480    -302900.000
    298.150    461.4707 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22300.000
-3.486280460D+03 0.000000000D+00 8.644374370D+00 1.088065032D-02 5.040262220D-07
 0.000000000D+00 0.000000000D+00              -3.950736400D+04-2.968661932D+01
ALI3(L)         Liquid. TPIS 1996 pt1 p193-5,115 pt2 p155.
 1 tpis96 AL  1.00I   3.00    0.00    0.00    0.00 2  407.6949480    -302900.000
    461.470   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       22300.000
 0.000000000D+00 0.000000000D+00 1.455287203D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.913903150D+04-5.670488781D+01
ALN(cr)         Hexagonal. TPIS 1996 pt1 p202 pt2 p163.
 2 tpis96 AL  1.00N   1.00    0.00    0.00    0.00 1   40.9882780    -319000.000
    100.000    300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3870.000
 3.654741530D+03 0.000000000D+00-2.148600451D+00 2.744441314D-02-2.763366825D-05
 0.000000000D+00 0.000000000D+00              -3.868948290D+04 7.733969220D+00
    300.000   1800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3870.000
-1.801549340D+05 0.000000000D+00 5.525280504D+00 4.025492783D-04 0.000000000D+00
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 0.000000000D+00 0.000000000D+00              -4.063616530D+04-3.018829926D+01
ALN(L)          Liquid. TPIS 1996 pt1 p202 pt2 p163.
 2 tpis96 AL  1.00N   1.00    0.00    0.00    0.00 3   40.9882780    -319000.000
   1800.000   2700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3870.000
 0.000000000D+00 0.000000000D+00 4.491184688D+00 9.460569534D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.955518910D+04-2.338770283D+01
   2700.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3870.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.755928440D+04-4.598731266D+01
AL(OH)3(a)       Gibbsite. Gurvich TPIS 1996 pt1 p150 pt2 p114.
 1 tpis96 AL  1.00O   3.00H   3.00    0.00    0.00 1   78.0035580   -1293500.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12460.000
-2.376748819D+04 9.289791210D+02-1.532337335D+01 1.307578268D-01-2.205157141D-04
 1.567014467D-07 0.000000000D+00              -1.605485750D+05 6.795129010D+01
AL2O3(a)         Alpha,corundum. TPIS 1996 pt1 p134; pt2 p103.
 3 tpis96 AL  2.00O   3.00    0.00    0.00    0.00 1  101.9612760   -1675700.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10016.000
-5.391549970D+06 1.036676983D+05-8.173229150D+02 3.388258720D+00-7.512400360D-03
 8.659248820D-06-4.066085670D-09              -6.660134650D+05 4.235502230D+03
    500.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10016.000
-6.042087868D+05 0.000000000D+00 1.475480816D+01 8.272285438D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.079235447D+05-8.136029480D+01
   1200.000   2327.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10016.000
 0.000000000D+00 0.000000000D+00 1.293774378D+01 1.992781294D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.060787581D+05-6.966603728D+01
AL2O3(L)         Liquid. TPIS 1996 pt1 p134 pt2 p103.
 1 tpis96 AL  2.00O   3.00    0.00    0.00    0.00 3  101.9612760   -1675700.000
   2327.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10016.000
 0.000000000D+00 0.000000000D+00 1.959225499D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.027701571D+05-1.108590952D+02
AL2S3(a)         Hexagonal alpha. TPIS 1996 pt1 p201 pt2 p162.
 2 tpis96 AL  2.00S   3.00    0.00    0.00    0.00 1  150.1610760    -648500.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18630.440
 0.000000000D+00 0.000000000D+00-1.347810098D+00 8.478152110D-02-1.270516814D-04
 0.000000000D+00 0.000000000D+00              -8.024014680D+04 2.103644584D+00
    298.150   1273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18630.440
-1.943109095D+05 0.000000000D+00 1.417618116D+01 2.164890054D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.297075040D+04-6.845362098D+01
AL2S3(b)         Rhombohedral gamma. TPIS 1996 pt1 p201 pt2 p162.
 1 tpis96 AL  2.00S   3.00    0.00    0.00    0.00 3  150.1610760    -648500.000
   1273.000   1373.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18630.440
 0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.445251510D+04-8.466769750D+01
AL2S3(L)         Liquid. TPIS 1996 pt1 p201 pt2 p162.
 1 tpis96 AL  2.00S   3.00    0.00    0.00    0.00 4  150.1610760    -648500.000
   1373.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18630.440
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.114023330D+04-9.722848599D+01
AL2SiO5(an)
 2 J 9/67 AL  2.00SI  1.00O   5.00    0.00    0.00 1  162.0455760   -2592171.414
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-9.286634200D+00 1.347672000D-01-2.323700000D-04
 1.876091900D-07-5.738148300D-11              -3.132766400D+05 3.271585900D+01
   1000.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.735174200D+01 8.743813500D-03-3.708471800D-06
 1.068828300D-09-1.176395000D-13              -3.179415100D+05-9.173874400D+01
AL4C3(cr)        Hexagonal. TPIS 1996 pt1 p207 pt2 p168.
 2 tpis96 AL  4.00C   3.00    0.00    0.00    0.00 1  143.9582520    -206900.000
    100.000    300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16470.000
 4.384127580D+03 0.000000000D+00-5.803779650D+00 1.009595640D-01-1.158851541D-04
 0.000000000D+00 0.000000000D+00              -2.660263745D+04 1.884004031D+01
    300.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16470.000
-4.483607573D+05 0.000000000D+00 1.788920814D+01 4.024290066D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.190056250D+04-9.494910735D+01
AL6Si2O13(s)
 2 J 9/67 AL  6.00SI  2.00O  13.00    0.00    0.00 1  426.0524280   -6819432.111
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.103467100D+01 2.667564300D-01-4.152476300D-04
 3.137697200D-07-9.249759700D-11              -8.256587000D+05 3.225479100D+01
   1000.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.523836400D+01 2.766142400D-02-1.467551200D-05
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 3.888584800D-09-3.666048200D-13              -8.368641700D+05-2.373956500D+02
B(b)           Beta. JANAF Jun.1983. NASA TP-3287 1993.
 2 j 6/83 B   1.00    0.00    0.00    0.00    0.00 1   10.8110000         0.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        1214.000
 2.598259342D+05-4.770773050D+03 3.464124480D+01-1.287342209D-01 2.897864235D-04
-3.307265950D-07 1.500151011D-10              2.146946846D+04-1.830824723D+02
    600.000   2350.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        1214.000
-8.697700220D+02-8.050405960D+02 4.079712880D+00-6.423381350D-04 4.846017800D-07
-1.252780673D-10 1.335923595D-14              3.397919930D+03-2.505906587D+01
B(L)           liquid. JANAF Jun.1983. NASA TP-3287 1993.
 1 j 6/83 B   1.00    0.00    0.00    0.00    0.00 2   10.8110000         0.000
   2350.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        1214.000
 0.000000000D+00 0.000000000D+00 3.818625511D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              3.360603140D+03-2.073167308D+01
BN(cr)          Hexagonal,boron nitride. TPIS 1996 pt1 p103 pt2 p82.
 2 tpis96 B   1.00N   1.00    0.00    0.00    0.00 1   24.8177400   -251000.000
    200.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2628.425
 4.927312430D+05-6.086406850D+03 2.678226753D+01-4.529686640D-02 5.305526030D-05
-3.041114432D-08 6.795343860D-12              -2.413474891D+02-1.570534002D+02
   1200.000   3240.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2628.425
-8.394039490D+05 0.000000000D+00 6.231256640D+00-1.258688680D-05 2.018144787D-09
 0.000000000D+00 0.000000000D+00              -3.427269230D+04-3.687260910D+01
BN(L)           Liquid,boron nitride. TPIS 1996 pt1 p103 pt2 p82.
 1 tpis96 B   1.00N   1.00    0.00    0.00    0.00 2   24.8177400   -251000.000
   3240.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2628.425
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.023409980D+04-4.862382389D+01
B2O3(cr)         Hexagonal,diboron trioxide. TPIS 1996 pt1 p21 pt2 p16.
 1 tpis96 B   2.00O   3.00    0.00    0.00    0.00 1   69.6202000   -1273500.000
    100.000    723.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9301.499
-5.595297380D+04 1.311214190D+03-1.178535942D+01 7.702795250D-02-9.740126500D-05
 4.692119720D-08 1.804813810D-12              -1.599672923D+05 5.866759160D+01
B2O3(L)          Liquid,diboron trioxide. TPIS 1996 pt1 p21 pt2 p16.
 1 tpis96 B   2.00O   3.00    0.00    0.00    0.00 2   69.6202000   -1273500.000
    723.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9301.499
 3.774124994D+05 0.000000000D+00 1.528015481D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.562115789D+05-8.056094941D+01
B2S3(cr)         Monoclinic,diboron trisulfide.TPIS1996 pt1 p101 pt2 p80.
 1 tpis96 B   2.00S   3.00    0.00    0.00    0.00 1  117.8200000   -243000.000
    298.150    840.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17200.400
-9.430501617D+04 0.000000000D+00 1.190088171D+01 8.711277033D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.347775180D+04-5.890696350D+01
B2S3(L)          Liquid,diboron trisulfide. TPIS 1996 pt1 p101 pt2 p80.
 1 tpis96 B   2.00S   3.00    0.00    0.00    0.00 2  117.8200000   -243000.000
    840.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17200.400
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.921234633D+04-8.268126136D+01
B3O3H3(cr)
 2 J 3/65 B   3.00H   3.00O   3.00    0.00    0.00 1   83.4550200   -1262312.999
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.159513730D+00-7.066833500D-03 9.249246940D-05
-1.028339050D-07 3.501505710D-11              -1.545696300D+05-2.752540350D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.284705170D+01 9.195813220D-02-8.106094360D-05
 3.273228400D-08-5.016119480D-12              -1.511097220D+05 7.015361500D+01
B4C(cr)          Hexagonal,tetraboron carbide.TPIS 1996 pt1 p111 pt2 p89.
 2 tpis96 B   4.00C   1.00    0.00    0.00    0.00 1   55.2547000    -62000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5611.469
-3.582115390D+07 6.748884130D+05-5.160630080D+03 2.049973510D+01-4.453648770D-02
 5.049831300D-05-2.340979136D-08              -3.040618105D+06 2.693617477D+04
    500.000   2743.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5611.469
-5.772904970D+05 0.000000000D+00 1.274373364D+01 5.718209610D-05 1.287030822D-06
 0.000000000D+00 0.000000000D+00              -1.320621763D+04-7.266962500D+01
B4C(cr)          Liquid,tetraboron carbide. JANAF June 1983.
 1 tpis96 B   4.00C   1.00    0.00    0.00    0.00 2   55.2547000    -62000.000
   2743.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5611.469
 0.000000000D+00 0.000000000D+00 1.635454164D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.250553215D+03-9.163227046D+01
Ba(cr)           Crystal. Alcock JPCRD v22 n1 1993 p1.
 2 srd 93 BA  1.00    0.00    0.00    0.00    0.00 1  137.3270000         0.000
    80.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6906.992
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-1.121413050D+03 0.000000000D+00 2.794031160D+00 3.089779190D-03-8.812305240D-06
 1.741533780D-08 0.000000000D+00                -9.306838000D+02-9.109787140D+00
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6906.992
 0.000000000D+00 0.000000000D+00 2.773344430D+00 2.037522360D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.174338100D+02-8.909706260D+00
Ba(L)           Liquid. Alcock JPCRD v22 n1 1993 p1.
 1 srd 93 BA  1.00    0.00    0.00    0.00    0.00 2  137.3270000         0.000
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6906.992
 0.000000000D+00 0.000000000D+00 4.810866790D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.920623810D+02-2.000275710D+01
BaBr2(cr)        Rhombic. TPIS 1996 pt1 p578 pt2 p438.
 1 tpis96 BA  1.00BR  2.00    0.00    0.00    0.00 1  297.1350000    -752000.000
    298.000   1130.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19000.460
-7.817658527D+03 0.000000000D+00 8.433088661D+00 2.644894287D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.310239840D+04-3.084013513D+01
BaBr2(L)         Liquid. TPIS 1996 pt1 p578 pt2 p438.
 1 tpis96 BA  1.00BR  2.00    0.00    0.00    0.00 2  297.1350000    -752000.000
   1130.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19000.460
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.227494300D+04-5.391493900D+01
BaCO3(a)         CrIII,rhombic. TPIS 1996 pt1 p588 pt2 p446.
 2 tpis96 BA  1.00C   1.00O   3.00    0.00    0.00 1  197.3359000   -1214000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16510.460
-2.877181104D+07 5.413510470D+05-4.125297560D+03 1.638620098D+01-3.558188760D-02
 4.031953330D-05-1.867325900D-08                -2.581769925D+06 2.154826876D+04
    500.000   1083.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16510.460
-4.578261377D+05 0.000000000D+00 1.897622349D+01-1.614166078D-02 1.493894409D-05
 0.000000000D+00 0.000000000D+00                -1.526176829D+05-9.306389650D+01
BaCO3(b)         CrII,hexagonal. TPIS 1996 pt1 p588 pt2 p446.
 1 tpis96 BA  1.00C   1.00O   3.00    0.00    0.00 3  197.3359000   -1214000.000
   1083.000   1233.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16510.460
 0.000000000D+00 0.000000000D+00 1.900292380D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.534042929D+05-9.996568172D+01
BaCO3(c)         CrI,cubic. TPIS 1996 pt1 p588 pt2 p446.
 1 tpis96 BA  1.00C   1.00O   3.00    0.00    0.00 4  197.3359000   -1214000.000
   1233.000   1828.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16510.460
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.533520950D+05-1.013948007D+02
BaCO3(L)         Liquid. TPIS 1996 pt1 p588 pt2 p446.
 1 tpis96 BA  1.00C   1.00O   3.00    0.00    0.00 5  197.3359000   -1214000.000
   1828.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16510.460
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.496405113D+05-1.032798247D+02
BaCL2(a)         CrII,rhombic. TPIS 1996 pt1 p574 pt2 p435.
 2 tpis96 BA  1.00CL  2.00    0.00    0.00    0.00 1  208.2324000    -855200.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16700.460
-7.376444120D+04 1.806760784D+03-1.415837573D+01 1.391571933D-01-4.179089240D-04
 6.207438290D-07-3.577305500D-10                -1.127273901D+05 7.349900590D+01
    500.000   1198.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16700.460
 7.096028509D+02 0.000000000D+00 8.343245723D+00 2.300676769D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.054434434D+05-3.333989736D+01
BaCL2(b)         CrI,cubic. TPIS 1996 pt1 p574 pt2 p435.
 1 tpis96 BA  1.00CL  2.00    0.00    0.00    0.00 3  208.2324000    -855200.000
   1198.000   1234.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16700.460
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.105803253D+05-8.137880037D+01
BaCL2(L)         Liquid. TPIS 1996 pt1 p574 pt2 p435.
 1 tpis96 BA  1.00CL  2.00    0.00    0.00    0.00 4  208.2324000    -855200.000
   1234.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16700.460
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.054088841D+05-6.099987667D+01
BaF2(a)          CrIII,cubic. TPIS 1996 pt1 p567 pt2 p431.
 2 tpis96 BA  1.00F   2.00    0.00    0.00    0.00 1  175.3238064   -1206000.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14440.460
 1.441693954D+05-4.606283760D+03 5.412180390D+01-2.221460987D-01 5.733095130D-04
-7.321844990D-07 3.715051400D-10                -1.283756240D+05-2.649277473D+02
    500.000   1240.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14440.460
-2.180525371D+04 0.000000000D+00 7.730461567D+00 3.587703906D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.475854552D+05-3.364924914D+01
BaF2(b)          CrII. TPIS 1996 pt1 p567 pt2 p431.
 1 tpis96 BA  1.00F   2.00    0.00    0.00    0.00 3  175.3238064   -1206000.000
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   1240.000   1480.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14440.460
 0.000000000D+00 0.000000000D+00 1.515423038D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.533548254D+05-8.153942783D+01
BaF2(c)          CrI. TPIS 1996 pt1 p567 pt2 p431.
 1 tpis96 BA  1.00F   2.00    0.00    0.00    0.00 4  175.3238064   -1206000.000
   1480.000   1641.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14440.460
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.535821388D+05-8.396607945D+01
BaF2(L)          Liquid. TPIS 1996 pt1 p567 pt2 p431.
 1 tpis96 BA  1.00F   2.00    0.00    0.00    0.00 5  175.3238064   -1206000.000
   1641.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14440.460
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.467045237D+05-6.129240287D+01
BaI2(cr)         Rhombic. TPIS 1996 pt1 p582 pt2 p441.
 2 tpis96 BA  1.00I   2.00    0.00    0.00    0.00 1  391.1359400    -606000.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19230.400
 1.510332529D+04-6.224807000D+02 1.545037842D+01-3.239437030D-02 9.253598890D-05
-1.251913725D-07 6.804559110D-11              -7.305629580D+04-6.364696150D+01
    500.000    984.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19230.400
-3.247335080D+02 0.000000000D+00 8.607723125D+00 2.399780624D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.555873070D+04-2.989160688D+01
BaI2(L)          Liquid. TPIS 1996 pt1 p582 pt2 p441.
 1 tpis96 BA  1.00I   2.00    0.00    0.00    0.00 3  391.1359400    -606000.000
    984.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19230.400
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.611264840D+04-5.863183475D+01
BaH2(a)          CrII,rhombic TPIS 1996 pt1 p556 pt2 p424.
 1 tpis96 BA  1.00H   2.00    0.00    0.00    0.00 1  139.3428800    -190000.000
    298.150    871.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9100.474
 0.000000000D+00 0.000000000D+00 4.530874339D+00 3.359308005D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.435180761D+04-1.923955725D+01
BaH2(b)          CrI,rhombic TPIS 1996 pt1 p556 pt2 p424.
 1 tpis96 BA  1.00H   2.00    0.00    0.00    0.00 2  139.3428800    -190000.000
    871.000   1473.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9100.474
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.589536064D+04-4.267585539D+01
BaH2(L)          Liquid TPIS 1996 pt1 p556 pt2 p424.
 1 tpis96 BA  1.00H   2.00    0.00    0.00    0.00 3  139.3428800    -190000.000
   1473.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9100.474
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.359720958D+04-4.414413915D+01
BaO(cr)          Cubic TPIS 1996 pt1 p547 pt2 p418.
 3 tpis96 BA  1.00O   1.00    0.00    0.00    0.00 1  153.3264000    -548000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
-3.734308680D+06 7.030482670D+04-5.334141930D+02 2.143135900D+00-4.664219600D-03
 5.294704440D-06-2.456512761D-09              -3.833163320D+05 2.789047565D+03
    500.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
-7.551858137D+04 0.000000000D+00 6.798957485D+00-1.205482945D-03 7.325747398D-07
 0.000000000D+00 0.000000000D+00              -6.814216420D+04-3.017618534D+01
   1400.000   2246.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
 1.380021192D+07 0.000000000D+00-1.685992319D+01 1.166250326D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.704906000D+04 1.274565988D+02
BaO(L)           Liquid TPIS 1996 pt1 p547 pt2 p418.
 1 tpis96 BA  1.00O   1.00    0.00    0.00    0.00 3  153.3264000    -548000.000
   2246.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9962.459
 0.000000000D+00 0.000000000D+00 1.001863008D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.861430250D+04-5.267326797D+01
Ba(OH)2(b)       CrII,rhombic TPIS 1996 pt1 p558 pt2 p427.
 1 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 1  171.3416800    -940600.000
    100.000    519.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16148.440
 5.078717800D+04-1.641996937D+03 1.964278489D+01-3.730614630D-02 1.039952734D-04
-8.659369050D-08 2.282290989D-11              -1.085585521D+05-9.701503650D+01
Ba(OH)2(a)       CrI,rhombic TPIS 1996 pt1 p558 pt2 p427.
 1 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 2  171.3416800    -940600.000
    519.000    681.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16148.440
 0.000000000D+00 0.000000000D+00 1.491368704D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.176117467D+05-7.252241184D+01
Ba(OH)2(L)       Liquid TPIS 1996 pt1 p558 pt2 p427.
 1 tpis96 BA  1.00O   2.00H   2.00    0.00    0.00 3  171.3416800    -940600.000
    681.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16148.440
 0.000000000D+00 0.000000000D+00 1.659749041D+01 0.000000000D+00 0.000000000D+00
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 0.000000000D+00 0.000000000D+00              -1.168340700D+05-8.068104197D+01
BaS(cr)          Cubic. TPIS 1996 pt1 p584 pt2 p443.
 2 tpis96 BA  1.00S   1.00    0.00    0.00    0.00 1  169.3930000    -470000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10820.450
 3.369786470D+05-6.138740230D+03 4.922553770D+01-1.599274620D-01 3.314481350D-04
-3.600847800D-07 1.611281388D-10              -3.028248993D+04-2.539125160D+02
    500.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10820.450
-2.050631967D+04 0.000000000D+00 5.920852822D+00 8.307164223D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.839868930D+04-2.466233780D+01
BaS(L)           Liquid. TPIS 1996 pt1 p584 pt2 p443.
 1 tpis96 BA  1.00S   1.00    0.00    0.00    0.00 3  169.3930000    -470000.000
   2500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10820.450
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.356075540D+04-3.627577743D+01
BaSO4(a)         CrII,rhombic. TPIS 1996 pt1 p587 pt2 p445.
 2 tpis96 BA  1.00S   1.00O   4.00    0.00    0.00 1  233.3906000   -1470000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19180.440
-1.712286968D+07 3.212789860D+05-2.441820133D+03 9.713067900D+00-2.105021811D-02
 2.383101570D-05-1.103328957D-08              -1.624343960D+06 1.276058048D+04
    500.000   1423.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19180.440
-2.747004935D+05 0.000000000D+00 1.352094110D+01 6.200004570D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.820275447D+05-6.454315519D+01
BaSO4(b)         CrI,cubic. TPIS 1996 pt1 p587 pt2 p445.
 1 tpis96 BA  1.00S   1.00O   4.00    0.00    0.00 3  233.3906000   -1470000.000
   1423.000   1853.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19180.440
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.842091207D+05-1.050884025D+02
BaSO4(L)         Liquid. TPIS 1996 pt1 p587 pt2 p435.
 1 tpis96 BA  1.00S   1.00O   4.00    0.00    0.00 4  233.3906000   -1470000.000
   1853.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19180.440
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.793982539D+05-1.024921441D+02
Be(a)            Alpha Crystal. Alcock JPCRD v22 no1 1993 p1.
 2 srd 93 BE  1.00    0.00    0.00    0.00    0.00 1    9.0121820         0.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 3.532378940D+03 0.000000000D+00-1.827528020D+00 1.895481510D-02-2.121592250D-05
 0.000000000D+00 0.000000000D+00              -9.832146860D+01 6.866894110D+00
    298.150   1543.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
-7.064757880D+04 0.000000000D+00 2.550360750D+00 6.848268870D-04 1.157013460D-07
 0.000000000D+00 0.000000000D+00              -1.028803670D+03-1.399471510D+01
Be(b)            Beta Crystal. Alcock JPCRD v22 no1 1993 p1.
 1 srd 93 BE  1.00    0.00    0.00    0.00    0.00 2    9.0121820         0.000
   1543.000   1563.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 0.000000000D+00 0.000000000D+00 3.608150090D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.524497790D+02-2.002895770D+01
Be(L)            Liquid. Modified Alcock JPCRD v22 n1 1993 p1.
 1 srd 93 BE  1.00    0.00    0.00    0.00    0.00 3    9.0121820         0.000
   1563.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 0.000000000D+00 0.000000000D+00 3.545608820D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               2.074755800D+02-1.895341260D+01
BeAL2O4(s)
 2 J12/79 BE  1.00AL  2.00O   4.00    0.00    0.00 1  126.9728580   -2300807.894
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-8.054738000D+00 1.135724000D-01-1.878272800D-04
 1.480685700D-07-4.480727800D-11              -2.779804400D+05 2.713571900D+01
   1000.000   2146.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.026555900D+01-1.046664900D-02 2.304395400D-05
-1.549368300D-08 3.602494000D-12              -2.833630100D+05-1.074722200D+02
BeAL2O4(L)
 1 J12/79 BE  1.00AL  2.00O   4.00    0.00    0.00 2  126.9728580         0.000
   2146.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.963629100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.805698200D+05-1.711695400D+02
BeBr2(cr)        Cr,rhombic. TPIS 1996 pt1 p376 pt2 p301.
 1 tpis96 BE  1.00BR  2.00    0.00    0.00    0.00 1  168.8201820    -358000.000
    298.150    781.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14900.000
-1.296528599D+05 0.000000000D+00 9.544519160D+00 8.967455689D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.637767130D+04-4.238810553D+01
BeBr2(L)         Liquid.TPIS 1996 pt1 p376 pt2 p301.
 1 tpis96 BE  1.00BR  2.00    0.00    0.00    0.00 2  168.8201820    -358000.000
    781.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14900.000
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 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.571223050D+04-5.534538359D+01
BeCO3(cr)        TPIS 1996 pt1 p385 pt2 p310.
 1 tpis96 BE  1.00C   1.00O   3.00    0.00    0.00 1   69.0210820   -1045000.000
    298.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9200.480
-3.688732108D+05 0.000000000D+00 1.057428520D+01 4.670148932D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.302813975D+05-5.746109667D+01
BeCL2(a)         Cr,rhombic. TPIS 1996 pt1 p370 pt2 p296.
 1 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 1   79.9175820    -496200.000
    200.000    676.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11420.000
-9.696336540D+05 1.653841300D+04-1.120322868D+02 4.343457410D-01-8.234422230D-04
 7.967601960D-07-3.089202126D-10              -1.372167152D+05 5.981191760D+02
BeCL2(b)         CrI. TPIS 1996 pt1 p370 pt2 p296.
 1 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 2   79.9175820    -496200.000
    676.000    688.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11420.000
 0.000000000D+00 0.000000000D+00 8.056999150D+00 2.516083329D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.169505530D+04-3.701517264D+01
BeCL2(L)         Liquid.TPIS 1996 pt1 p370 pt2 p296.
 1 tpis96 BE  1.00CL  2.00    0.00    0.00    0.00 3   79.9175820    -496200.000
    688.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11420.000
 0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.212751630D+04-5.342382325D+01
BeF2(a)          CrII,hexagonal.TPIS 1996 pt1 p364 pt2 p292.
 1 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 1   47.0089884   -1027000.000
    200.000    493.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8468.000
 3.082582728D+05-5.000745390D+03 3.049066381D+01-5.416146720D-02 5.846680620D-05
 0.000000000D+00 0.000000000D+00              -1.011928897D+05-1.687961461D+02
BeF2(b)          CrI,hexagonal.TPIS 1996 pt1 p364 pt2 p292.
 1 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 2   47.0089884   -1027000.000
    493.000    823.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8468.000
 0.000000000D+00 0.000000000D+00 5.652527930D+00 3.986885577D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.252903029D+05-2.679700109D+01
BeF2(L)          Liquid.TPIS 1996 pt1 p364 pt2 p292.
 1 tpis96 BE  1.00F   2.00    0.00    0.00    0.00 3   47.0089884   -1027000.000
    823.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8468.000
-1.882035141D+06 0.000000000D+00 1.234468417D+01-1.836548396D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.310986361D+05-6.898102574D+01
BeI2(cr)         Cr,rhombic. TPIS 1996 pt1 p379 pt2 p304.
 1 tpis96 BE  1.00I   2.00    0.00    0.00    0.00 1  262.8211220    -191000.000
    298.150    763.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15200.000
-1.443741122D+05 0.000000000D+00 1.007828483D+01 3.371214900D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.647594661D+04-4.378170625D+01
BeI2(L)          Liquid.TPIS 1996 pt1 p379 pt2 p304.
 1 tpis96 BE  1.00I   2.00    0.00    0.00    0.00 2  262.8211220    -191000.000
    763.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15200.000
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.551070377D+04-5.349837990D+01
BeO(a)           CrII,hexagonal. TPIS 1996 pt1 p348 pt2 p278.
 2 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 1   25.0115820    -609400.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2837.000
 2.047701543D+05-2.981173217D+03 1.385643338D+01-1.581697711D-02 2.353849388D-05
-1.941029834D-08 6.520569610D-12              -5.922219190D+04-8.231113660D+01
   1000.000   2373.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2837.000
 1.024057237D+06 1.937465590D+03-2.170213872D+00 6.700940070D-03-1.829092628D-06
 2.757893870D-10-2.712743027D-14              -8.276808970D+04 1.896607400D+01
BeO(b)           CrI,tetragonal. TPIS 1996 pt1 p348 pt2 p278.
 1 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 2   25.0115820    -609400.000
   2373.000   2851.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2837.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.674474850D+04-3.937528813D+01
BeO(L)           Liquid. TPIS 1996 pt1 p348 pt2 p278.
 1 tpis96 BE  1.00O   1.00    0.00    0.00    0.00 3   25.0115820    -609400.000
   2851.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        2837.000
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.600243170D+04-6.253805395D+01
Be(OH)2(b)       Rhombic,beta.TPIS 1996 pt1 p359 pt2 p289.
 2 tpis96 BE  1.00O   2.00H   2.00    0.00    0.00 1   43.0268620    -905700.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8293.440
-2.821507074D+07 5.306026240D+05-4.050124700D+03 1.608285663D+01-3.491136410D-02
 3.956008990D-05-1.833019806D-08              -2.495097922D+06 2.114570392D+04
    500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8293.440
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-4.549275904D+05 0.000000000D+00 1.198362862D+01 2.034996650D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.141192354D+05-6.597431876D+01
BeS(cr)          Cr,cubic. TPIS 1996 pt1 p381 pt2 p306.
 1 tpis96 BE  1.00S   1.00    0.00    0.00    0.00 1   41.0781820    -236000.000
    298.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5500.480
-1.061156941D+05 0.000000000D+00 4.876054031D+00 1.363880734D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.025444334D+04-2.469606404D+01
BeSO4(a)         CrIII,tetr. TPIS 1996 pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00    0.00    0.00 1  105.0757820   -1200000.000
    200.000    861.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12970.000
 9.674052850D+05-1.525976877D+04 9.078019340D+01-2.151323890D-01 3.405813330D-04
-2.623119799D-07 8.137303080D-11              -7.417050650D+04-5.024380540D+02
BeSO4(b)         CrII,rhombic. TPIS 1996 pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00    0.00    0.00 2  105.0757820   -1200000.000
    861.000    912.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12970.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.508085273D+05-9.670719282D+01
BeSO4(c)         CrI,cubic. TPIS 1996 pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00    0.00    0.00 3  105.0757820   -1200000.000
    912.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12970.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.505559568D+05-9.643025148D+01
BeSO4(L)         Liquid. TPIS 1996 pt1 p383 pt2 p308.
 1 tpis96 BE  1.00S   1.00O   4.00    0.00    0.00 4  105.0757820   -1200000.000
   1400.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12970.000
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.498343268D+05-9.591480146D+01
Be2C(s)
 2 BAR 73 BE  2.00C   1.00    0.00    0.00    0.00 1   30.0350640    -116986.029
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.437417000D+00 2.569453800D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.550732400D+04-2.408612100D+01
   1000.000   2400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.437417000D+00 2.569453800D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.550732400D+04-2.408612100D+01
Be2C(L)
 1 BAR 73 BE  2.00C   1.00    0.00    0.00    0.00 2   30.0350640    -116986.029
   2400.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.107089700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.496964100D+04-6.577511600D+01
Be3N2(a)         CrII,cubic. TPIS 1996 pt1 p384 pt2 p309.
 2 tpis96 BE  3.00N   2.00    0.00    0.00    0.00 1   55.0500260    -588000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7124.000
 6.443341310D+05-9.239880870D+03 4.211333200D+01-4.513325350D-02 3.232975930D-05
 0.000000000D+00 0.000000000D+00              -2.674920290D+04-2.511544265D+02
    500.000   1673.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7124.000
-2.278465381D+05 4.432191420D+02 1.376274664D+00 3.225384830D-02-2.704770612D-05
 8.116575420D-09-6.682374890D-14              -7.562743780D+04-1.197625563D+01
Be3N2(b)         CrI,hexagonal. TPIS 1996 pt1 p384 pt2 p309.
 1 tpis96 BE  3.00N   2.00    0.00    0.00    0.00 2   55.0500260    -588000.000
   1673.000   2473.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7124.000
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.850942150D+04-1.016302777D+02
Be3N2(L)         Liquid. TPIS 1996 pt1 p384 pt2 p309.
 1 tpis96 BE  3.00N   2.00    0.00    0.00    0.00 3   55.0500260    -588000.000
   2473.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7124.000
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.182303830D+04-1.169540588D+02
Br2(cr)          Bromine Rhombic. TPIS 1989 v1, pt 2, p314. JANAF, 6/82.
 1 tpis89 BR  2.00    0.00    0.00    0.00    0.00 1  159.8080000         0.000
    200.000    265.9007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24520.000
 1.079338540D+06-9.504318700D+03-8.951502070D+01 1.645929070D+00-8.633183930D-03
 2.007102780D-05-1.744155310D-08               5.482480050D+04 2.476936180D+02
Br2(L)           Bromine Liquid.  TPIS 1989 v1, pt 2, p314. JANAF, 6/82.
 2 tpis89 BR  2.00    0.00    0.00    0.00    0.00 2  159.8080000         0.000
    265.900    332.5037 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24520.000
 4.023495180D+06-3.952532570D+04-2.246976760D+01 1.958462760D+00-1.015816590D-02
 2.161796540D-05-1.708373620D-08               2.134322580D+05-2.532613200D+02
    332.503   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24520.000
 0.000000000D+00 0.000000000D+00 9.056686430D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.699855620D+03-3.329349960D+01
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C(gr)          Graphite. TRC Tables VC,UC,TC-1000-1002,Apr 30,1983.
 3 X 4/83 C   1.00    0.00    0.00    0.00    0.00 1   12.0107000         0.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        1053.500
 1.132856760D+05-1.980421677D+03 1.365384188D+01-4.636096440D-02 1.021333011D-04
-1.082893179D-07 4.472258860D-11                8.943859760D+03-7.295824740D+01
    600.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        1053.500
 3.356004410D+05-2.596528368D+03 6.948841910D+00-3.484836090D-03 1.844192445D-06
-5.055205960D-10 5.750639010D-14                1.398412456D+04-4.477183040D+01
   2000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        1053.500
 2.023105106D+05-1.138235908D+03 3.700279500D+00-1.833807727D-04 6.343683250D-08
-7.068589480D-12 3.335435980D-16                5.848134850D+03-2.350925275D+01
Ca(a)          Alpha Crystal. Alcock JPCRD v22 n1 1993 p1.
 2 srd 93 CA  1.00    0.00    0.00    0.00    0.00 1   40.0780000         0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5782.945
-8.385644720D+05 1.765286050D+04-1.464598170D+02 6.316166740D-01-1.329219360D-03
 1.117756580D-06 0.000000000D+00                -7.826284690D+04 7.549642720D+02
    298.150    716.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5782.945
-6.262296480D+05 8.185565830D+03-4.063986690D+01 1.203863930D-01-1.801843350D-04
 1.443177100D-07-4.731328580D-11                -4.064340460D+04 2.315315500D+02
Ca(b)          Beta Crystal. Alcock JPCRD v22 n1 1993 p1.
 1 srd 93 CA  1.00    0.00    0.00    0.00    0.00 2   40.0780000         0.000
    716.000   1115.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5782.945
 0.000000000D+00 0.000000000D+00 5.701117680D+00-5.810564900D-03 4.022125180D-06
 0.000000000D+00 0.000000000D+00                -1.516739110D+03-2.607571900D+01
Ca(L)          Liquid. Alcock JPCRD v22 n1 1993 p1.
 1 srd 93 CA  1.00    0.00    0.00    0.00    0.00 3   40.0780000         0.000
   1115.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5782.945
 0.000000000D+00 0.000000000D+00 4.570323450D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.822188080D+02-2.119876990D+01
CaBr2(cr)        Rhombic TPIS 1996 pt1 p473 pt2 p368.
 1 tpis96 CA  1.00BR  2.00    0.00    0.00    0.00 1  199.8860000    -683800.000
    298.150   1015.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17000.490
-2.826384237D+04 0.000000000D+00 8.872561342D+00 1.586623866D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.505243950D+04-3.554898721D+01
CaBr2(L)         Liquid TPIS 1996 pt1 p473 pt2 p368.
 1 tpis96 CA  1.00BR  2.00    0.00    0.00    0.00 2  199.8860000    -683800.000
   1015.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17000.490
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.390932270D+04-5.231487518D+01
CaCO3(cr)        Hexagonal TPIS 1996 pt1 p483 pt2 p376.
 2 tpis96 CA  1.00C   1.00O   3.00    0.00    0.00 1  100.0869000   -1206600.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14480.499
-1.329862425D+07 2.500517168D+05-1.907177167D+03 7.616666270D+00-1.655870860D-02
 1.879382277D-05-8.720713270D-09                -1.271058215D+06 9.957497560D+03
    500.000   1603.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14480.499
-2.583555736D+05 0.000000000D+00 1.197256363D+01 3.263812299D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.497009803D+05-5.961133653D+01
CaCO3(L)         Liquid TPIS 1996 pt1 p483 pt2 p376.
 1 tpis96 CA  1.00C   1.00O   3.00    0.00    0.00 3  100.0869000   -1206600.000
   1603.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14480.499
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.526719277D+05-1.052847193D+02
CaCL2(cr)        Rhombic. TPIS 1996 pt1 p467 pt2 p365.
 2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 1  110.9834000    -795800.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15300.460
 6.000206010D+03-4.466152170D+02 8.199988600D+00 2.374917562D-02-1.002337283D-04
 1.782027609D-07-1.141389034D-10                -9.606057780D+04-3.912159570D+01
    500.000   1048.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15300.460
-3.018818908D+04 0.000000000D+00 8.644766799D+00 1.529735366D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.845880750D+04-3.684266549D+01
CaCL2(L)         Liquid. TPIS 1996 pt1 p467 pt2 p365.
 1 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 3  110.9834000    -795800.000
   1048.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15300.460
 2.661491778D+06 0.000000000D+00 1.078355790D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.391818610D+04-4.566953897D+01
CaF2(a)          CrII,cubic.TPIS 1996 pt1 p461 pt2 p361.
 3 tpis96 CA  1.00F   2.00    0.00    0.00    0.00 1   78.0748064   -1228000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11640.000
-9.875281260D+05 1.337426670D+04-6.261903110D+01 1.617894422D-01-1.271795719D-04
 0.000000000D+00 0.000000000D+00                -2.146045473D+05 3.617287210D+02
    500.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11640.000
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-6.961842180D+06 4.692065010D+04-1.157708151D+02 1.655025287D-01-1.108459197D-04
 3.213053720D-08 0.000000000D+00              -4.101016540D+05 7.419533450D+02
   1000.000   1424.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11640.000
 1.438558077D+09 7.852955040D+05-1.342916213D+04 2.192783112D+01-1.383442475D-02
 3.122877330D-06 0.000000000D+00              2.168972069D+06 7.823794920D+04
CaF2(b)          CrI,cubic.TPIS 1996 pt1 p461 pt2 p361.
 1 tpis96 CA  1.00F   2.00    0.00    0.00    0.00 2   78.0748064   -1228000.000
   1424.000   1691.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11640.000
 1.535768139D+08 0.000000000D+00-1.699774473D+02 7.733123360D-02 3.585714680D-07
 0.000000000D+00 0.000000000D+00              1.356828739D+05 1.185723820D+03
CaF2(L)          Liquid.TPIS 1996 pt1 p461 pt2 p361.
 1 tpis96 CA  1.00F   2.00    0.00    0.00    0.00 3   78.0748064   -1228000.000
   1691.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11640.000
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.479539740D+05-5.967665213D+01
CaH2(a)          CrII,rhombic TPIS 1996 pt1 p449 pt2 p354.
 1 tpis96 CA  1.00H   2.00    0.00    0.00    0.00 1   42.0938800    -177000.000
    298.150   1053.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6770.474
 0.000000000D+00 0.000000000D+00 3.599731073D+00 4.465566822D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.255982511D+04-1.686197756D+01
CaH2(b)          CrI,cubic TPIS 1996 pt1 p449 pt2 p354.
 1 tpis96 CA  1.00H   2.00    0.00    0.00    0.00 2   42.0938800    -177000.000
   1053.000   1273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6770.474
 0.000000000D+00 0.000000000D+00 8.298745206D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.422633646D+04-4.409678633D+01
CaH2(L)          Liquid TPIS 1996 pt1 p449 pt2 p354.
 1 tpis96 CA  1.00H   2.00    0.00    0.00    0.00 3   42.0938800    -177000.000
   1273.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6770.474
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.249899474D+04-4.717727797D+01
CaI2(cr)         Hexagonal TPIS 1996 pt1 p476 pt2 p371.
 2 tpis96 CA  1.00I   2.00    0.00    0.00    0.00 1  293.8869400    -536400.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17970.499
-1.811328452D+06 3.127451814D+04-2.136599007D+02 8.328705880D-01-1.721725832D-03
 1.878967812D-06-8.440013400D-10              -2.101977983D+05 1.142802698D+03
    500.000   1056.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17970.499
-6.638996165D+03 0.000000000D+00 8.652825001D+00 2.284560365D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.721736780D+04-3.254333551D+01
CaI2(L)          Liquid TPIS 1996 pt1 p476 pt2 p371.
 1 tpis96 CA  1.00I   2.00    0.00    0.00    0.00 3  293.8869400    -536400.000
   1056.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17970.499
 0.000000000D+00 0.000000000D+00 1.238798197D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.485425310D+04-5.137218163D+01
CaO(cr)          Cubic TPIS 1996 pt1 p442 pt2 p348.
 2 tpis96 CA  1.00O   1.00    0.00    0.00    0.00 1   56.0774000    -634920.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6750.499
-4.775526940D+06 9.037711420D+04-6.944320810D+02 2.802477174D+00-6.129403220D-03
 6.982167800D-06-3.247543840D-09              -4.829411430D+05 3.619046320D+03
    500.000   3172.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6750.499
-1.459376440D+05 0.000000000D+00 7.174205094D+00-1.959947129D-03 1.291116374D-06
-2.077091735D-10 0.000000000D+00              -7.891525080D+04-3.658562837D+01
CaO(L)           Liquid TPIS 1996 pt1 p442 pt2 p348.
 1 tpis96 CA  1.00O   1.00    0.00    0.00    0.00 3   56.0774000    -634920.000
   3172.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6750.499
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.991857230D+04-5.908720013D+01
Ca(OH)2(cr)      Hexagonal TPIS 1996 pt1 p454 pt2 p357.
 2 tpis96 CA  1.00O   2.00H   2.00    0.00    0.00 1   74.0926800    -985900.000
    100.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14160.490
-2.058838935D+05 6.172554490D+03-7.499750990D+01 5.012182400D-01-1.423348682D-03
 1.994984415D-06-1.095038067D-09              -1.452026205D+05 3.552445040D+02
    500.000   1023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14160.490
-1.245413139D+05 0.000000000D+00 1.073593032D+01 3.982435525D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.223707243D+05-5.302395390D+01
Ca(OH)2(L)       Liquid TPIS 1996 pt1 p454 pt2 p357.
 1 tpis96 CA  1.00O   2.00H   2.00    0.00    0.00 3   74.0926800    -985900.000
   1023.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        14160.490
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.245191822D+05-9.860760364D+01
CaS(cr)          Cubic TPIS 1996 pt1 p478 pt2 p373.
 2 tpis96 CA  1.00S   1.00    0.00    0.00    0.00 1   72.1440000    -475000.000
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    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9010.499
 4.758681130D+06-8.840702110D+04 6.675047510D+02-2.576855161D+00 5.527281760D-03
-6.202901900D-06 2.852128154D-09                3.401344700D+05-3.494344760D+03
    500.000   2800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9010.499
-1.428827435D+04 0.000000000D+00 5.567375588D+00 1.006673875D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.888163400D+04-2.530572359D+01
CaS(L)          Liquid TPIS 1996 pt1 p478 pt2 p373.
 1 tpis96 CA  1.00S   1.00    0.00    0.00    0.00 3   72.1440000    -475000.000
   2800.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9010.499
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.348566620D+04-3.924995523D+01
CaSO4(II)        Rhombic TPIS 1996 pt1 p481 pt2 p375.
 2 tpis96 CA  1.00S   1.00O   4.00    0.00    0.00 1  136.1416000   -1434000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17200.499
-1.361977472D+07 2.584929291D+05-1.984800641D+03 7.969448170D+00-1.736805219D-02
 1.974370111D-05-9.168768090D-09                -1.334631522D+06 1.035139350D+04
    500.000   1473.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17200.499
-2.983940124D+05 0.000000000D+00 1.359671225D+01 5.857230312D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.777846313D+05-6.802481458D+01
CaSO4(I)         Cubic TPIS 1996 pt1 p481 pt2 p375.
 1 tpis96 CA  1.00S   1.00O   4.00    0.00    0.00 3  136.1416000   -1434000.000
   1473.000   1733.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17200.499
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.798298668D+05-1.045004358D+02
CaSO4(L)         Liquid TPIS 1996 pt1 p481 pt2 p375.
 1 tpis96 CA  1.00S   1.00O   4.00    0.00    0.00 4  136.1416000   -1434000.000
   1733.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17200.499
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.764622601D+05-1.025572120D+02
Cd(cr)          Cadmium Crystal. CODATA 1989, p223.
 1 coda89 CD  1.00    0.00    0.00    0.00    0.00 1  112.4110000        0.000
    100.000    594.2587 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6247.000
 1.375273140D+05-3.221589850D+03 3.121905280D+01-1.226136690D-01 2.838880270D-04
-3.286883630D-07 1.520469610D-10                1.302806940D+04-1.551324020D+02
Cd(L)           Cadmium Liquid. CODATA 1989, p223.
 1 coda89 CD  1.00    0.00    0.00    0.00    0.00 2  112.4110000        0.000
    594.258   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6247.000
 0.000000000D+00 0.000000000D+00 3.596122920D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.220394770D+02-1.323298160D+01
Co(a)           Cobalt Alpha Crystal. JANAF, SEPT. 1967.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 1   58.9332000        0.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
-8.650414060D+05 1.461861080D+04-9.968931130D+01 3.793451210D-01-7.798095020D-04
 8.551200040D-07-3.888996480D-10                -6.794739000D+04 5.305430680D+02
    500.000    700.1007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
-9.856619810D+05 6.806164130D+03-1.517922420D+01 2.230314250D-02-9.001300570D-06
 0.000000000D+00 0.000000000D+00                -3.844851400D+04 1.012032700D+02
Co(b)           Cobalt Beta below Lambda transition. JANAF,9/1967.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 2   58.9332000        0.000
    700.100    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
 0.000000000D+00 0.000000000D+00 2.125113810D+00 2.218475450D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.197709750D+02-8.944546660D+00
    800.000   1394.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
-1.402743650D+09 8.165151370D+06-1.964940010D+04 2.502806370D+01-1.778064400D-02
 6.679858190D-06-1.035836070D-09                -4.620353590D+07 1.250995880D+05
Co(b)           Cobalt Beta above Lambda transition. JANAF,9/1967.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 3   58.9332000        0.000
   1394.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
 0.000000000D+00 0.000000000D+00 3.070869280D+02-2.155485170D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.139294060D+05-1.913103400D+03
   1400.000   1768.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
 1.638463110D+09-4.011240680D+06 3.699045810D+03-1.516406030D+00 2.339096860D-04
 0.000000000D+00 0.000000000D+00                 2.632689000D+07-2.734045280D+04
Co(L)           Cobalt Liquid. JANAF, SEPT. 1967.
 1 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 4   58.9332000        0.000
   1768.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4771.000
 0.000000000D+00 0.000000000D+00 4.871122890D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.764314840D+02-2.448435110D+01
Cr(cr)
 1 J 6/73 CR  1.00    0.00    0.00    0.00    0.00 1   51.9961000        0.000
    200.000    311.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 7.848260240D+00-1.162760200D-01 8.123692510D-04
-2.308070860D-06 2.353281420D-09              -8.980139460D+02-2.757331390D+01
Cr(cr)          Chromium Crystal. Below lambda trans. JANAF. June 1973.
 1 j 6/73 CR  1.00    0.00    0.00    0.00    0.00 1   51.9961000         0.000
    200.000    311.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4057.000
 8.050183280D+05-1.339702210D+04 8.272693050D+01-2.075649580D-01 2.008567710D-04
 0.000000000D+00 0.000000000D+00               6.181694490D+04-4.559518770D+02
Cr(cr)          Chromium Crystal. Above lambda trans. JANAF. June 1973.
 2 j 6/73 CR  1.00    0.00    0.00    0.00    0.00 2   51.9961000         0.000
    311.500   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4057.000
-2.534457120D+05 3.119436960D+03-1.358453440D+01 4.323599580D-02-5.624137260D-05
 3.652931660D-08-8.973350170D-12              -1.606575840D+04 7.858123410D+01
   1000.000   2130.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4057.000
-3.001490030D+07 1.262933320D+05-2.136852190D+02 1.935375970D-01-9.411602750D-05
 2.442072870D-08-2.603463620D-12              -7.573543950D+05 1.440200410D+03
Cr(L)           Chromium Liquid. JANAF. June 1973.
 1 j 6/73 CR  1.00    0.00    0.00    0.00    0.00 3   51.9961000         0.000
   2130.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4057.000
 0.000000000D+00 0.000000000D+00 4.730284770D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               5.755633770D+02-2.453179000D+01
CrN(s)
 2 J12/73 CR  1.00N   1.00    0.00    0.00    0.00 1   66.0028400    -117293.818
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.715290400D+00-2.377537200D-02 5.256101500D-05
-4.839074700D-08 1.627075700D-11              -1.632342200D+04-4.573005000D+01
   1000.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.694453900D+00 5.301169000D-04 2.270582900D-07
-8.148325400D-11 1.080379600D-14              -1.583600200D+04-2.813170400D+01
Cr2N(s)
 2 J12/73 CR  2.00N   1.00    0.00    0.00    0.00 1  117.9989400    -125532.096
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.030338800D+00 3.400644100D-02-6.152494600D-05
 5.314254800D-08-1.676952100D-11              -1.676831300D+04-1.160069800D+01
   1000.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.098418500D+00 1.853361100D-03 1.422730600D-06
-5.589639000D-10 6.930711000D-14              -1.768480100D+04-3.914747200D+01
Cr2O3(s)
 2 J12/73 CR  2.00O   3.00    0.00    0.00    0.00 1  151.9904000   -1135094.145
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.933277300D+01-1.020738500D-01 2.360110300D-04
-2.257801900D-07 7.779928900D-11              -1.424040600D+05-1.357428100D+02
   1000.000   2603.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.401223500D+01 1.382397800D-03-2.377922600D-07
 1.699508500D-10-3.770585700D-14              -1.409821700D+05-7.110156900D+01
Cr2O3(L)
 1 J12/73 CR  2.00O   3.00    0.00    0.00    0.00 2  151.9904000         0.000
   2603.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.887110500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.336949800D+05-9.996147000D+01
Cs(cr)          Cesium Crystal. CODATA, 1989, p263.
 1 coda89 CS  1.00    0.00    0.00    0.00    0.00 1  132.9054500         0.000
    100.000    301.5907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7711.000
 6.519841250D+04-1.756639050D+03 1.999681070D+01-6.938328730D-02 1.093682540D-04
 0.000000000D+00 0.000000000D+00               6.382890730D+03-9.338251450D+01
Cs(L)           Cesium Liquid. CODATA, 1989, p263.
 2 coda89 CS  1.00    0.00    0.00    0.00    0.00 2  132.9054500         0.000
    301.590   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7711.000
-4.218327690D+04-1.743103180D+01 5.702124720D+00-5.113669890D-03 3.201407010D-06
-1.765747120D-10 4.822129370D-14              -1.290949810D+03-2.031407580D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7711.000
-7.266594990D+05 3.006769060D+03 1.696418950D-01 2.912560320D-04 1.768808250D-07
 7.730274520D-10-8.902165320D-14              -1.923761690D+04 1.641003740D+01
CsCL(a)
 1 J 6/68 CS  1.00CL  1.00    0.00    0.00    0.00 1  168.3581500    -442845.665
    300.000    743.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.545340000D+00 2.380583400D-03 8.357033000D-07
-9.957164000D-10 3.805480300D-13              -5.502653500D+04-2.016426000D+01
CsCL(b)
 1 J 6/68 CS  1.00CL  1.00    0.00    0.00    0.00 2  168.3581500         0.000
    743.000    918.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.161073700D+00-1.762356800D-03-2.250851600D-07
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 3.930731700D-09-2.345234100D-12              -5.548043100D+04-3.394139600D+01
CsCL(L)
 2 J 6/68 CS  1.00CL  1.00    0.00    0.00    0.00 3  168.3581500         0.000
   918.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.309745200D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.503116100D+04-4.081013300D+01
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.309745200D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.503116100D+04-4.081013300D+01
CsF(s)
 1 J 6/68 CS  1.00F   1.00    0.00    0.00    0.00 1  151.9038532    -554685.846
   300.000    976.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.648999300D+00 1.871139800D-03 6.624238200D-07
-6.308487100D-10 1.869233900D-13              -6.848510200D+04-2.214995900D+01
CsF(L)
 2 J 6/68 CS  1.00F   1.00    0.00    0.00    0.00 2  151.9038532         0.000
   976.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.907161700D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.806681700D+04-3.991277400D+01
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.907161700D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.806681700D+04-3.991277400D+01
CsOH(b)          Beta.  JPCRD v26 n4,1997 p1031.
 2 g 8/97 CS  1.00O   1.00H   1.00    0.00    0.00 1  149.9127900    -416200.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14103.000
-1.070491244D+06 2.726790967D+04-2.447999195D+02 9.717566950D-01-1.304183626D-03
 0.000000000D+00 0.000000000D+00              -1.676915176D+05 1.260979156D+03
   298.150    498.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14103.000
 2.988510447D+05 0.000000000D+00-5.599488124D+00 4.758933479D-02-3.982976748D-05
 0.000000000D+00 0.000000000D+00              -4.914854260D+04 3.370083195D+01
CsOH(c)          Gamma. JPCRD v26 n4,1997 p1031.
 1 g 8/97 CS  1.00O   1.00H   1.00    0.00    0.00 3  149.9127900    -416200.000
   498.200    615.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14103.000
 0.000000000D+00 0.000000000D+00 8.743750383D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.198053970D+04-3.591737929D+01
CsOH(L)          Liquid.JPCRD v26 n4,1997 p1031.
 1 g 8/97 CS  1.00O   1.00H   1.00    0.00    0.00 4  149.9127900    -416200.000
   615.500   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14103.000
 0.000000000D+00 0.000000000D+00 1.022309192D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.195536080D+04-4.389810453D+01
Cs2SO4(II)
 1 J 6/79 CS  2.00S   1.00O   4.00    0.00    0.00 1  361.8745000   -1442695.595
   300.000    940.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.978930700D+00 1.265088400D-01-2.955320600D-04
 3.320730800D-07-1.310499100D-10              -1.762335200D+05 1.518574700D+01
Cs2SO4(I)
 2 J 6/79 CS  2.00S   1.00O   4.00    0.00    0.00 2  361.8745000         0.000
   940.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.734983600D+00 1.861960000D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.715413900D+05 1.373704600D-01
  1000.000   1278.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.723272200D-02 3.135403600D-02-1.130053100D-05
 3.328310800D-09 0.000000000D+00              -1.702116300D+05 2.483998800D+01
Cs2SO4(L)
 1 J 6/79 CS  2.00S   1.00O   4.00    0.00    0.00 3  361.8745000         0.000
  1278.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.485919800D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.777619800D+05-1.166574400D+02
Cu(cr)           Copper Cubic Crystal. CODATA, 1989, p226.
 1 coda89 CU  1.00    0.00    0.00    0.00    0.00 1   63.5460000         0.000
   200.000   1358.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5004.000
-2.455775170D+04 1.648069280D+02 2.080947100D+00 2.639078400D-03-2.714101480D-06
 1.402865050D-09-9.724323270D-14              -1.737851010D+03-8.133166580D+00
Cu(L)            Copper Liquid. CODATA, 1989, p226.
 1 coda89 CU  1.00    0.00    0.00    0.00    0.00 2   63.5460000         0.000
  1358.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5004.000
 0.000000000D+00 0.000000000D+00 3.944910760D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.111013780D+02-1.836065770D+01
CuF(s)
 2 J12/77 CU  1.00F   1.00    0.00    0.00    0.00 1   82.5444032    -280337.300
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 4.442128800D+00 7.966907600D-03-7.280731100D-06
 2.763777300D-09-2.731884200D-13              -3.533616800D+04-1.958517000D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.321550600D+00 4.854983200D-03-3.544004800D-06
 1.110902300D-09-1.245371600D-13              -3.552171500D+04-2.390264300D+01
CuF2(s)
 2 J12/77 CU  1.00F   2.00    0.00    0.00    0.00 1  101.5428064    -538916.630
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.387367600D+00 1.439710900D-02-8.621349700D-06
-1.983044600D-09 2.689674000D-12              -6.668558500D+04-1.958056100D+01
   1000.000   1109.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.355767600D+00 1.491350800D-02-6.399519300D-06
 0.000000000D+00 0.000000000D+00              -6.561062200D+04-7.162675700D+00
CuF2(L)
 1 J12/77 CU  1.00F   2.00    0.00    0.00    0.00 2  101.5428064         0.000
   1109.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.207750700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.348799800D+04-5.673037000D+01
CuO(s)
 2 J12/77 CU  1.00O   1.00    0.00    0.00    0.00 1   79.5454000    -156065.450
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.840386600D-01 2.415885200D-02-4.389414200D-05
 3.758618100D-08-1.208827500D-11              -1.978838200D+04-5.472388000D+00
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.025812400D+00 2.542407700D-03-1.376829400D-06
 5.349283100D-10-7.966428100D-14              -2.043328100D+04-2.437669500D+01
CuO2H2(s)
 2 J 6/66 CU  1.00O   2.00H   2.00    0.00    0.00 1   97.5606800    -450377.208
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.045118500D+01 1.345820500D-03 8.660233900D-06
-6.809234900D-09 7.443585900D-13              -5.740686500D+04-4.723880300D+01
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.673078700D+00 1.038576200D-02-4.699484100D-06
-5.029251300D-10 5.359316000D-13              -5.723038200D+04-3.936616100D+01
CuSO4(s)
 2 J 6/66 CU  1.00S   1.00O   4.00    0.00    0.00 1  159.6096000    -770006.799
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.301916600D+00 3.701232100D-02-2.899080400D-05
 4.531404500D-09 2.638844500D-12              -9.499362100D+04-1.546587800D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.131453600D+01 1.405035200D-02-1.006356800D-05
 3.720422100D-09-5.280591400D-13              -9.699820800D+04-5.625469000D+01
Cu2O(s)
 2 J12/77 CU  2.00O   1.00    0.00    0.00    0.00 1  143.0914000    -170709.678
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.383246600D+00 2.295417600D-02-3.954230400D-05
 3.402040100D-08-1.104380900D-11              -2.227315700D+04-1.353071300D+01
   1000.000   1516.7207 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.475564100D+01-1.587665700D-02 1.497119300D-05
-4.484026400D-09 4.055600500D-13              -2.506506800D+04-7.054187700D+01
Cu2O(L)
 1 J12/77 CU  2.00O   1.00    0.00    0.00    0.00 2  143.0914000         0.000
   1516.720   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.201712000D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.925238700D+04-5.688686600D+01
Cu2O5S(s)
 2 J 6/66 CU  2.00O   5.00S   1.00    0.00    0.00 1  239.1550000    -927626.899
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.525717800D+00 7.220595800D-02-9.785566500D-05
 6.543249900D-08-1.674445300D-11              -1.147864600D+05-1.319611200D+01
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.601163400D+01 1.942466800D-02-1.844825100D-05
 1.118720400D-08-2.611198300D-12              -1.176162000D+05-7.872748900D+01
Fe(a)          Iron below Lambda transition. JANAF, MAR.1978.
 3 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 1   55.8450000         0.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       4507.000
 1.349559940D+04-7.802009540D+02 9.438756970D+00-2.521186010D-02 5.348852000D-05
-5.097531900D-08 1.993105380D-11               2.415718860D+03-4.748269040D+01
    500.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       4507.000
 3.542934690D+06-2.447087250D+04 6.560869360D+01-7.043770040D-02 3.180990490D-05
 0.000000000D+00 0.000000000D+00               1.345024530D+05-4.133691000D+02
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   800.000   1042.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 2.277422620D+09-5.694572230D+06-5.624964090D+03 3.185945470D+01-3.850131890D-02
 1.870814650D-05-3.017627050D-09                4.007254040D+07 1.621757760D+04
Fe(a)          Iron above Lambda transition. JANAF, MAR.1978.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 2   55.8450000         0.000
   1042.000   1184.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 2.481963970D+08 0.000000000D+00-5.594448520D+02 3.271764180D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.467615930D+05 3.669233740D+03
Fe(c)          Iron Gamma Crystal. JANAF, MAR.1978.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 3   55.8450000         0.000
   1184.000   1665.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 9.135010080D+08-3.056481710D+06 3.974073180D+03-2.422054440D+00 6.065114910D-04
 1.242318820D-08-2.203150860D-11                1.906636000D+07-2.792308700D+04
Fe(d)          Iron Delta Crystal. JANAF, MAR.1978.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 4   55.8450000         0.000
   1665.000   1809.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
-3.469127030D+08 0.000000000D+00 7.096069130D+02-5.472910000D-01 1.196569310D-04
 0.000000000D+00 0.000000000D+00               -8.089869360D+05-4.570050840D+03
Fe(L)          Iron Liquid. JANAF, MAR.1978.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 5   55.8450000         0.000
   1809.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4507.000
 0.000000000D+00 0.000000000D+00 5.535383320D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.270474900D+03-2.948096830D+01
FeC5O5(L)
 2 J 3/78 FE  1.00C   5.00O   5.00    0.00    0.00 1  195.8955000    -766109.877
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.811845000D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.005248300D+05-1.196654100D+02
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.811845000D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.005248300D+05-1.196654100D+02
FeCL2(s)
 1 J12/70 FE  1.00CL  2.00    0.00    0.00    0.00 1  126.7504000    -341840.884
    300.000    950.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.112227100D+00 1.108695300D-02-1.707274200D-05
 1.351581700D-08-4.136503600D-12               -4.360098500D+04-2.899405500D+01
FeCL2(L)
 2 J12/70 FE  1.00CL  2.00    0.00    0.00    0.00 2  126.7504000         0.000
    950.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.228886300D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.110982100D+04-5.319305700D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.228886300D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.110982100D+04-5.319305700D+01
FeCL3(s)
 1 J 6/65 FE  1.00CL  3.00    0.00    0.00    0.00 1  162.2031000    -399405.000
    200.000    577.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-7.395568550D+00 2.026084340D-01-8.445059230D-04
 1.592866020D-06-1.079893210D-09               -5.001446640D+04 2.444509350D+01
FeCL3(L)
 2 J 6/65 FE  1.00CL  3.00    0.00    0.00    0.00 2  162.2031000    -399405.000
    577.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.610312700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.841352780D+04-6.757589900D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.610312700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.841352780D+04-6.757589900D+01
FeO(s)
 2 J 6/65 FE  1.00O   1.00    0.00    0.00    0.00 1   71.8444000    -272037.027
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.319547500D+00 2.209659100D-03 1.072177500D-06
-2.792972900D-09 1.332073300D-12               -3.440716500D+04-2.368603400D+01
   1000.000   1650.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.831648900D+00 1.427515600D-03-9.320814300D-08
-6.599776300D-12-2.251214300D-14               -3.456690200D+04-2.644699000D+01
FeO(L)
 1 J 6/65 FE  1.00O   1.00    0.00    0.00    0.00 2   71.8444000         0.000
   1650.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.202248200D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.384861500D+04-4.007912900D+01
Fe(OH)2(s)
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 2 J 6/66 FE  1.00O   2.00H   2.00    0.00    0.00 1   89.8596800    -574058.558
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.009121800D+01 4.452314100D-03 4.066685500D-06
-4.009452500D-09 2.394716400D-13               -7.227768800D+04-4.840003400D+01
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.403180800D+00 1.198174200D-02-1.495761100D-06
-5.052635900D-09 2.003711100D-12               -7.159226600D+04-3.467326700D+01
Fe(OH)3(s)
 2 J 6/66 FE  1.00O   3.00H   3.00    0.00    0.00 1  106.8670200    -832627.354
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.411683600D+00 3.268246200D-02-2.239381500D-05
 2.864679200D-09 2.262232100D-12               -1.027183400D+05-2.133101400D+01
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.022392600D+00 1.642013500D-02-1.236937800D-07
-6.819283800D-09 2.327690700D-12               -1.032133600D+05-3.793402000D+01
FeS(a)
 1 J 9/77 FE  1.00S   1.00    0.00    0.00    0.00 1   87.9110000    -101818.255
    300.000    411.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.897762700D+01-1.095428200D-01 2.218601600D-04
 0.000000000D+00 0.000000000D+00               -1.499524200D+04-7.812543500D+01
FeS(b)
 1 J 9/77 FE  1.00S   1.00    0.00    0.00    0.00 2   87.9110000         0.000
    411.000    598.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.702850500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.468973800D+04-4.208210200D+01
FeS(c)
 2 J 9/77 FE  1.00S   1.00    0.00    0.00    0.00 3   87.9110000         0.000
    598.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.372417600D+00 9.416205900D-04-1.582986400D-05
 1.838088100D-08-5.770706700D-12               -1.458168500D+04-4.514151600D+01
   1000.000   1463.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.683048300D+00 3.676510400D-02-5.218227400D-05
 3.160717000D-08-6.412604100D-12               -1.149868400D+04 1.623912400D+01
FeS(L)
 1 J 9/77 FE  1.00S   1.00    0.00    0.00    0.00 4   87.9110000         0.000
   1463.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.523280600D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.016423700D+04-3.197093000D+01
FeSO4(s)
 2 J 6/66 FE  1.00S   1.00O   4.00    0.00    0.00 1  151.9086000    -928877.319
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.505768400D+00 3.702970100D-02-2.903353100D-05
 4.577858900D-09 2.620208700D-12               -1.141625000D+05-1.522324100D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.160892900D+01 1.380469700D-02-9.812638000D-06
 3.608781100D-09-5.097627900D-13               -1.161918600D+05-5.647781700D+01
FeS2(s)
 2 J 9/77 FE  1.00S   2.00    0.00    0.00    0.00 1  119.9770000    -171549.187
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.034566300D-01 4.267468400D-02-8.403062600D-05
 7.630144100D-08-2.543231600D-11               -2.204592700D+04-5.545639300D+00
   1000.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-8.851532000D+01 3.274893100D-01-4.105743900D-04
 2.292814600D-07-4.776441500D-11               -4.651247600D+02 4.417304500D+02
Fe2O3(s)
 2 J 6/65 FE  2.00O   3.00    0.00    0.00    0.00 1  159.6882000    -825315.197
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-7.703784300D+00 1.364747100D-01-3.290565500D-04
 3.815047800D-07-1.631028500D-10               -1.008007600D+05 2.529208500D+01
   1000.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.049753000D+01-4.613159600D-02 3.182640600D-05
-8.922633100D-09 8.465541700D-13               -1.131762700D+05-2.163508800D+02
Fe2S3O12(s)
 2 J 6/66 FE  2.00S   3.00O  12.00    0.00    0.00 1  399.8808000   -2583054.471
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.111695500D+01 8.370677800D-02-4.136507500D-05
-2.527922200D-08 2.104143500D-11               -3.172978200D+05-4.928875000D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.911443800D+01 1.179632700D-02-3.387101400D-08
-2.297039900D-09 6.410198600D-13               -3.247826200D+05-1.940042900D+02
Fe3O4(s)
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 2 J 6/65 FE  3.00O   4.00    0.00    0.00    0.00 1  231.5326000   -1119932.370
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.619814800D+01-1.743797600D-01 5.247567300D-04
-5.423821900D-07 1.799620200D-10              -1.413873000D+05-1.555668300D+02
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.413372000D+01 4.159222600D-05-2.633149200D-08
 6.603509400D-12-5.692468000D-16              -1.412105200D+05-1.200641200D+02
Ga(cr)          Gallium Rhombic Crystal. TPIS 1996 pt1 p209;pt2 p169.
 1 tpis96 GA  1.00    0.00    0.00    0.00    0.00 1   69.7230000         0.000
    100.000    302.9207 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5640.000
 1.665524651D+03-1.667535996D+02 3.860876380D+00-1.325442179D-03 2.405494396D-06
 0.000000000D+00 0.000000000D+00              -1.577791876D+02-1.730178030D+01
Ga(L)           Gallium Liquid. TPIS 1996 pt1 p209;pt2 p169.
 1 tpis96 GA  1.00    0.00    0.00    0.00    0.00 2   69.7230000         0.000
    302.920   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5640.000
 2.846830421D+04 0.000000000D+00 3.135362156D+00-3.620177256D-05 2.898547239D-08
 0.000000000D+00 0.000000000D+00              -1.716496723D+02-1.053717280D+01
GaBr3(cr)        TPIS 1996 pt1 p242; pt2 p195.
 1 tpis96 GA  1.00BR  3.00    0.00    0.00    0.00 1  309.4350000    -387000.000
    298.150    397.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       25000.000
 0.000000000D+00 0.000000000D+00 3.563409028D+00 2.798433101D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.885137800D+04-6.997495329D+00
GaBr3(L)         Liquid. TPIS 1996 pt1 p242;pt2 p195.
 1 tpis96 GA  1.00BR  3.00    0.00    0.00    0.00 2  309.4350000    -387000.000
    397.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       25000.000
 0.000000000D+00 0.000000000D+00 1.544288238D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.990695050D+04-6.330801668D+01
GaCL3(cr)        Triclinic. TPIS 1996 pt1 p234; pt2 p188.
 1 tpis96 GA  1.00CL  3.00    0.00    0.00    0.00 1  176.0811000    -527000.000
    298.150    351.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20000.000
 0.000000000D+00 0.000000000D+00 2.725476306D+00 2.958442530D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.551070110D+04-8.232857519D+00
GaCL3(L)         Liquid. TPIS 1996 pt1 p234;pt2 p188.
 1 tpis96 GA  1.00CL  3.00    0.00    0.00    0.00 2  176.0811000    -527000.000
    351.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       20000.000
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.599449360D+04-5.489418092D+01
GaF3(cr)         Hexagonal. TPIS 1996 pt1 p226; pt2 p181.
 1 tpis96 GA  1.00F   3.00    0.00    0.00    0.00 1  126.7182096   -1175000.000
    298.150   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16700.000
 0.000000000D+00 0.000000000D+00 9.361585950D+00 4.503211855D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.443105216D+05-4.313509369D+01
GaI3(cr)         Rhombic. TPIS 1996 pt1 p249; pt2 p202.
 1 tpis96 GA  1.00I   3.00    0.00    0.00    0.00 1  450.4364100    -218000.000
    298.150    485.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       29000.000
 0.000000000D+00 0.000000000D+00 6.461715723D+00 1.866676449D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.897546082D+04-1.772605384D+01
GaI3(L)          Liquid. TPIS 1996 pt1 p249;pt2 p202.
 1 tpis96 GA  1.00I   3.00    0.00    0.00    0.00 2  450.4364100    -218000.000
    485.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       29000.000
 0.000000000D+00 0.000000000D+00 1.656140891D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.012686264D+04-6.793170105D+01
Ga2O3(cr)        Monoclinic. TPIS 1996 pt1 p219; pt2 p176.
 2 tpis96 GA  2.00O   3.00    0.00    0.00    0.00 1  187.4442000   -1091000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14550.000
-1.515635939D+07 2.787922412D+05-2.090093764D+03 8.236854680D+00-1.771414598D-02
 1.991804320D-05-9.167934200D-09              -1.391968792D+06 1.094221304D+04
    500.000   2080.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14550.000
-2.857534599D+05 0.000000000D+00 1.375883846D+01 1.799504721D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.363570445D+05-7.032081677D+01
Ga2O3(L)         Liquid. TPIS 1996 pt1 p219;pt2 p176.
 1 tpis96 GA  2.00O   3.00    0.00    0.00    0.00 3  187.4442000   -1091000.000
   2080.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14550.000
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.317078351D+05-1.026657694D+02
Ge(cr)          Germanium Cubic. TPIS 1991, v2, pt1, p308, pt2 p268.
 2 tpis91 GE  1.00    0.00    0.00    0.00    0.00 1   72.6100000         0.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4636.360
-2.396503710D+05 3.150568730D+03-1.333939590D+01 3.647993850D-02-2.942101330D-05
 0.000000000D+00 0.000000000D+00              -1.613881310D+04 7.939201580D+01
    400.000   1211.4007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4636.360
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-1.888241350D+04 0.000000000D+00 2.898173040D+00 3.591659390D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.433863850D+02-1.298669710D+01
Ge(L)          Germanium Liquid. TPIS 1991, v2, pt1, p308, pt2 p268.
 1 tpis91 GE  1.00    0.00    0.00    0.00    0.00 2   72.6100000         0.000
   1211.400   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4636.360
 0.000000000D+00 0.000000000D+00 3.319498080D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               3.278996640D+03-1.185992950D+01
GeO2(II)        Germanium Dioxide Tetragonal Rutile,TPIS,1991.
 2 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 1  104.6088000    -580200.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7230.400
-1.362061010D+04 0.000000000D+00 1.390091028D+00 1.608814892D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.095682740D+04-8.017483700D+00
    298.150   1308.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7230.400
-2.763121338D+05 0.000000000D+00 9.404643208D+00-1.212218158D-03 1.110107511D-06
 0.000000000D+00 0.000000000D+00              -7.346830070D+04-5.004997052D+01
GeO2(I)         Germanium Dioxide Hexagonal alpha-quartz,TPIS,1991.
 1 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 3  104.6088000    -580200.000
   1308.000   1388.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7230.400
-1.535267863D+05 0.000000000D+00 7.481860025D+00 1.711465859D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.994652970D+04-3.711331960D+01
GeO2(L)         Germanium Dioxide Tetragonal liquid,TPIS,1991.
 1 tpis91 GE  1.00O   2.00    0.00    0.00    0.00 4  104.6088000    -580200.000
   1388.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7230.400
 0.000000000D+00 0.000000000D+00 9.441326067D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.883837870D+04-4.738551165D+01
GeS(cr)         Germanium Sulfide Crystal(II).TPIS,1991.
 2 tpis91 GE  1.00S   1.00    0.00    0.00    0.00 1  104.6760000     -75348.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9657.400
-1.753890915D+04 0.000000000D+00 4.967049230D+00 3.277123440D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.074763864D+04-2.138030847D+01
    298.150    931.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9657.400
 0.000000000D+00 0.000000000D+00 5.015328624D+00 2.453542061D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.066660187D+04-2.131118286D+01
GeS(L)          Germanium Sulfide Liquid.TPIS,1991.
 1 tpis91 GE  1.00S   1.00    0.00    0.00    0.00 3  104.6760000     -75348.000
    931.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9657.400
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.874413010D+03-3.707715519D+01
GeS2(cr)        Germanium Disulfide Crystal(II).TPIS,1991.
 2 tpis91 GE  1.00S   2.00    0.00    0.00    0.00 1  136.7420000    -121500.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12750.300
-2.239538329D+04 0.000000000D+00 5.754200020D+00 8.048243800D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.676145505D+04-2.405323435D+01
    298.150   1113.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12750.300
-3.367606750D+04 0.000000000D+00 7.889821529D+00 1.310961199D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.713657615D+04-3.427587425D+01
GeS2(L)         Germanium Disulfide Liquid.TPIS,1991.
 1 tpis91 GE  1.00S   2.00    0.00    0.00    0.00 2  136.7420000    -121500.000
   1113.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12750.300
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.893876733D+04-6.006450099D+01
HBO2(cr)        Crystal,metaboric acid. TPIS 1996 pt1 p41 pt2 p25.
 1 tpis96 H   1.00B   1.00O   2.00    0.00    0.00 1   43.8177400    -804600.000
    298.150    509.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8460.200
 0.000000000D+00 0.000000000D+00 4.478916978D+00 7.045514408D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.841912440D+04-2.172637097D+01
HBO2(L)         Liquid, metaboric acid. TPIS 1996 pt1 p41 pt2 p25.
 1 tpis96 H   1.00B   1.00O   2.00    0.00    0.00 2   43.8177400    -804600.000
    509.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8460.200
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.993471070D+04-6.555326576D+01
H2O(s)          ICE. SANFORD GORDON, NASA TP-1906, 1982.
 1 g 8/89 H   2.00O   1.00    0.00    0.00    0.00 1   18.0152800    -299108.000
    200.000    273.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-3.897362880D+05 2.415022040D+03 6.094190680D+01-8.470311370D-01 4.477681170D-03
-1.065218620D-05 9.771898510D-09              -5.391506160D+04-2.075964810D+02
H2O(L)          COX ET.AL.,CODATA KEY VALUES FOR THERMODYNAMICS.1989.
 1 g 8/89 H   2.00O   1.00    0.00    0.00    0.00 2   18.0152800    -285830.000
    273.150    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13278.000
 8.721237810D+07-1.390875110D+06 9.157295320D+03-3.175963510D+01 6.138850760D-02
-6.267988650D-05 2.645363490D-08               6.433165230D+06-4.909853190D+04
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H2SO4(L)
 1 J 9/77 H   2.00S   1.00O   4.00    0.00    0.00 1   98.0794800    -814010.341
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.942152500D+00 2.178636900D-02 3.497445800D-06
-3.354885700D-09 1.169958600D-12              -1.018597900D+05-4.439869500D+01
H3BO3(cr)        Triclinic,orthoboric acid. TPIS 1996 pt1 p48 pt2 p31.
 1 tpis96 H   3.00B   1.00O   3.00    0.00    0.00 1   61.8330200   -1094800.000
    200.000    444.1007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13520.430
 2.370260101D+06-3.116426553D+04 1.488140666D+02-2.710868145D-01 2.274904549D-04
 0.000000000D+00 0.000000000D+00               1.950811769D+04-8.575441950D+02
H3BO3(L)         Liquid,orthoboric acid. TPIS 1996 pt1 p48 pt2 p31.
 1 tpis96 H   3.00B   1.00O   3.00    0.00    0.00 2   61.8330200   -1094800.000
    444.100   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13520.430
 0.000000000D+00 0.000000000D+00 2.164890054D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.367426553D+05-1.100910256D+02
H3PO4(cr)        Phosphoric acid. JPCRD v14 1985 Sup1 p1295.
 1 j12/71 H   3.00P   1.00O   4.00    0.00    0.00 1   97.9951810   -1284488.000
    200.000    315.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16980.000
 2.733365471D+03 0.000000000D+00 1.109347863D+00 4.129024570D-02-7.810353320D-06
 0.000000000D+00 0.000000000D+00              -1.565753156D+05-4.973473130D+00
H3PO4(L)         Phosphoric acid. JPCRD v14 1985 Sup1 p1295.
 1 j12/71 H   3.00P   1.00O   4.00    0.00    0.00 2   97.9951810   -1284488.000
    315.500   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       16980.000
 4.109081110D+04-4.410343500D+02 8.547791650D+00 3.198261330D-02 5.167529530D-06
-3.256216600D-09 8.323148740D-13              -1.543175380D+05-4.155398650D+01
Hg(cr)           Mercury Tetragonal Crystal. JANAF, Dec. 1961.
 1 j12/61 HG  1.00    0.00    0.00    0.00    0.00 1  200.5900000         0.000
    100.000    234.2907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9343.000
-3.184586680D+03 0.000000000D+00 3.464424870D+00-4.054864610D-03 1.766281130D-05
 0.000000000D+00 0.000000000D+00              -1.282454340D+03-1.132010160D+01
Hg(L)            Mercury Liquid. JANAF, Dec. 1961.
 2 j12/61 HG  1.00    0.00    0.00    0.00    0.00 2  200.5900000         0.000
    234.290    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9343.000
 1.058322370D+05-1.993821170D+03 1.880573750D+01-5.994669400D-02 1.228324830D-04
-1.293153160D-07 5.530725520D-11               7.916755300D+03-9.064853320D+01
    600.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9343.000
 7.913801540D+05-3.956304980D+03 1.106460790D+01-8.153922660D-03 4.970465690D-06
-1.510415510D-09 1.872034190D-13               2.213759860D+04-6.072429040D+01
HgBr2(s)
 1 J 3/62 HG  1.00BR  2.00    0.00    0.00    0.00 1  360.3980000    -169456.464
    300.000    514.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.282971400D+00 1.630236400D-03 3.422987900D-06
 7.096199200D-10-4.335386200D-12              -2.295243800D+04-2.734527600D+01
HgBr2(L)
 2 J 3/62 HG  1.00BR  2.00    0.00    0.00    0.00 2  360.3980000         0.000
    514.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.227879900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.250089800D+04-4.685121200D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.227879900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.250089800D+04-4.685121200D+01
HgO(s)
 1 J 6/62 HG  1.00O   1.00    0.00    0.00    0.00 1  216.5894000     -90786.065
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.417086600D+00 7.116057000D-03-1.489699600D-06
-4.491354800D-09 2.593792400D-12              -1.223327000D+04-1.303718500D+01
I2(cr)           Iodine Rhombic Crystal. TPIS 1989, v1, pt2, p315.
 1 tpis89 I   2.00    0.00    0.00    0.00    0.00 1  253.8089400         0.000
    200.000    386.7507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13196.000
-3.915902520D+06 9.175464720D+04-8.929786540D+02 4.685341330D+00-1.360919450D-02
 2.079243250D-05-1.295983020D-08              -3.926596480D+05 4.437381680D+03
I2(L)            Iodine Liquid. TPIS 1989, v1, pt2, p315.
 1 tpis89 I   2.00    0.00    0.00    0.00    0.00 2  253.8089400         0.000
    386.750   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13196.000
 0.000000000D+00 0.000000000D+00 9.568212680D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.204453820D+03-3.637326100D+01
In(cr)           Crystal TPIS 1996 pt 2  p207
 1 tpis96 IN  1.00    0.00    0.00    0.00    0.00 1  114.8180000         0.000
    100.000    429.7847 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6610.080
 8.511616870D+03-3.450470040D+02 6.838785170D+00-1.818530679D-02 4.122421420D-05
-2.960008730D-08 0.000000000D+00               4.580589980D+02-2.928914154D+01
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In(L)          Liquid  TPIS 1996 pt 2  p207
 1 tpis96 IN  1.00    0.00    0.00    0.00    0.00 2  114.8180000         0.000
   429.784   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6610.080
 5.092302493D+04 0.000000000D+00 3.302178962D+00-1.313366633D-04 6.037637816D-08
 0.000000000D+00 0.000000000D+00              -4.511517590D+02-1.075015830D+01
InBr(cr)        Rhombic TPIS 1996 pt1 p289; pt2 p232.
 1 tpis96 IN  1.00BR  1.00    0.00    0.00    0.00 0  194.7220000    -175000.000
   298.150    558.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12200.000
 0.000000000D+00 0.000000000D+00 4.633586345D+00 4.628534935D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.263476911D+04-1.455042037D+01
InBr(L)         Liquid TPIS 1996 pt1 p289; pt2 p232
 1 tpis96 IN  1.00BR  1.00    0.00    0.00    0.00 0  194.7220000    -175000.000
   558.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12200.000
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.222238473D+04-3.267500998D+01
InBr3(cr)       TPIS 1996 pt1 p292; pt2 p235.
 1 tpis96 IN  1.00BR  3.00    0.00    0.00    0.00 1  354.5300000    -399000.000
   298.150    693.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24500.000
 0.000000000D+00 0.000000000D+00 1.154114915D+01 2.436824299D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.153769860D+04-4.543581045D+01
InBr3(L)        Liquid TPIS 1996 pt1 p292; pt2 p235.
 1 tpis96 IN  1.00BR  3.00    0.00    0.00    0.00 2  354.5300000    -399000.000
   693.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24500.000
 0.000000000D+00 0.000000000D+00 1.623667540D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.107949370D+04-6.994831229D+01
InCL(crII)      Cubic TPIS 1996 pt1 p280; pt2 p224.
 1 tpis96 IN  1.00CL  1.00    0.00    0.00    0.00 0  150.2707000    -186500.000
   298.150    387.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12400.000
 0.000000000D+00 0.000000000D+00 5.163984408D+00 3.438567035D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.412314134D+04-1.842034240D+01
InCL(crI)       Rhombic TPIS 1996 pt1 p280; pt2 p224.
 1 tpis96 IN  1.00CL  1.00    0.00    0.00    0.00 0  150.2707000    -186500.000
   387.000    484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12400.000
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.441117035D+04-2.629006183D+01
InCL(L)         Liquid TPIS 1996 pt1 p280; pt2 p224
 1 tpis96 IN  1.00CL  1.00    0.00    0.00    0.00 0  150.2707000    -186500.000
   484.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12400.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.248971016D+04-2.917594080D+01
InCl3(cr)       Monoclinic TPIS 1996 pt1 p284; pt2 p227.
 1 tpis96 IN  1.00CL  3.00    0.00    0.00    0.00 1  221.1761000    -530000.000
   298.150    856.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21000.000
 0.000000000D+00 0.000000000D+00 1.093437857D+01 3.665158861D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.716697410D+04-4.631386948D+01
InCl3(L)        Liquid TPIS 1996 pt1 p284; pt2 p227.
 1 tpis96 IN  1.00CL  3.00    0.00    0.00    0.00 2  221.1761000    -530000.000
   856.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       21000.000
 0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.526246230D+04-6.056749656D+01
InF3(cr)        Hexagonal TPIS 1996 pt1 p274; pt2 p219.
 1 tpis96 IN  1.00F   3.00    0.00    0.00    0.00 1  171.8132096   -1190000.000
   298.150   1445.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19400.000
 0.000000000D+00 0.000000000D+00 9.751747247D+00 4.404348542D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.462265291D+05-4.364479594D+01
InF3(L)         Liquid TPIS 1996 pt1 p274; pt2 p219.
 1 tpis96 IN  1.00F   3.00    0.00    0.00    0.00 2  171.8132096   -1190000.000
  1445.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       19400.000
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.431278760D+05-7.826197980D+01
InI(cr)         Rhombic TPIS 1996 pt1 p296; pt2 p240
 1 tpis96 IN  1.00I   1.00    0.00    0.00    0.00 0  241.7224700    -102500.000
   200.000    637.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13354.000
-9.253976720D+04 1.215133840D+03-1.038882859D-02 1.368794477D-02-9.117964390D-06
 1.596277777D-09 1.519819589D-12              -2.009017203D+04 1.436598613D+01
InI(L)          Liquid TPIS 1996 pt1 p296; pt2 p240
 1 tpis96 IN  1.00I   1.00    0.00    0.00    0.00 0  241.7224700    -102500.000
   637.500   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13354.000
 0.000000000D+00 0.000000000D+00 8.443071209D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.331949891D+04-3.168475714D+01
InI2(crII)      TPIS 1996 pt1 p299; pt2 p242.
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 1 tpis96 IN  1.00I   2.00    0.00    0.00    0.00 0  368.6269400    -176000.000
    200.000    428.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19197.000
 2.657410907D+04 0.000000000D+00 6.946210170D+00 6.889884760D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.345592914D+04-2.056620828D+01
InI2(crI)        TPIS 1996 pt1 p299; pt2 p242.
 1 tpis96 IN  1.00I   2.00    0.00    0.00    0.00 0  368.6269400    -176000.000
    428.000    497.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19197.000
 0.000000000D+00 0.000000000D+00 1.080520680D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.438345996D+04-4.070950647D+01
InI2(L)          Liquid TPIS 1996 pt1 p299; pt2 p242.
 1 tpis96 IN  1.00I   2.00    0.00    0.00    0.00 0  368.6269400    -176000.000
    497.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19197.000
 0.000000000D+00 0.000000000D+00 1.379516051D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.444424767D+04-5.640525880D+01
InI3(cr)         Monoclinic TPIS 1996 pt1 p301; pt2 p244.
 1 tpis96 IN  1.00I   3.00    0.00    0.00    0.00 1  495.5314100    -224000.000
    296.000    480.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        29888.000
-1.888265213D+03 0.000000000D+00 1.096468704D+01 4.804492387D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.042985260D+04-3.708283570D+01
InI3(L)          Liquid TPIS 1996 pt1 p301; pt2 p244.
 1 tpis96 IN  1.00I   3.00    0.00    0.00    0.00 2  495.5314100    -224000.000
    480.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        29888.000
 0.000000000D+00 0.000000000D+00 1.652532741D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -3.031892811D+04-6.447232654D+01
In2O3(cr)        Cubic TPIS 1996 pt1 p267; pt2 p214.
 2 tpis96 IN  2.00O   3.00    0.00    0.00    0.00 0  277.6342000    -923000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16600.000
-9.503707350D+06 1.770907496D+05-1.344503703D+03 5.391303710D+00-1.171772659D-02
 1.329195789D-05-6.163943540D-09               -9.104733670D+05 7.021339210D+03
    500.000   2186.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16600.000
-2.719943809D+05 0.000000000D+00 1.461433085D+01 1.210173540D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.163340719D+05-7.291389772D+01
In2O3(L)         Liquid  TPIS 1996 pt2  p214
 1 tpis96 IN  2.00O   3.00    0.00    0.00    0.00 0  277.6342000    -923000.000
   2186.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16600.000
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.108089477D+05-1.000602622D+02
K(cr)            Potassium Cubic Crystal.  CODATA 1989, p257.
 1 coda89 K   1.00    0.00    0.00    0.00    0.00 1   39.0983000         0.000
    200.000    336.8607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7088.000
-1.022031740D+05 0.000000000D+00 1.333752010D+01-5.580990710D-02 9.013009050D-05
 0.000000000D+00 0.000000000D+00                -2.635062420D+03-5.615376490D+01
K(L)             Potassium Liquid.  CODATA 1989, p257.
 1 coda89 K   1.00    0.00    0.00    0.00    0.00 2   39.0983000         0.000
    336.860   2200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7088.000
-3.935792780D+03-4.547228660D+01 4.845242690D+00-3.083544870D-03 2.015547680D-06
-3.706132040D-11 5.032839710D-15               -8.075636970D+02-1.836640920D+01
KCN(s)
 1 J 3/66 K   1.00C   1.00N   1.00    0.00    0.00 1   65.1157400    -113473.603
    300.000    895.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.179972800D+00-1.401078200D-03 3.423772500D-06
-3.496173800D-09 1.305278000D-12               -1.604820100D+04-3.094452500D+01
KCN(L)
 2 J 3/66 K   1.00C   1.00N   1.00    0.00    0.00 2   65.1157400         0.000
    895.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.058130500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.522671700D+04-3.545408300D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.058130500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.522671700D+04-3.545408300D+01
KCL(s)
 2 J 3/66 K   1.00CL  1.00    0.00    0.00    0.00 1   74.5510000    -436694.011
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.393431100D+00 2.653524200D-03 9.607565500D-07
-5.025184300D-09 4.072122800D-12               -5.424838900D+04-2.159681400D+01
   1000.000   1044.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.915716900D+00-2.092727100D-03 4.731018200D-06
 7.015253700D-09-5.514609800D-12               -5.274706600D+04-1.014480000D+01
KCL(L)
 1 J 3/66 K   1.00CL  1.00    0.00    0.00    0.00 2   74.5510000         0.000
   1044.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 8.851806400D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.336947800D+04-4.001005900D+01
KF(s)
 2 J 6/69 K   1.00F   1.00    0.00    0.00    0.00 1   58.0967032    -568615.996
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.984397200D+00 3.594319000D-03-1.769640100D-06
-4.810614100D-10 1.028073000D-12              -7.001814900D+04-2.138450400D+01
   1000.000   1131.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.462778200D+00-6.405751200D-03 6.391326200D-08
 7.594958900D-09-3.359810400D-12              -7.124910700D+04-4.483180400D+01
KF(L)
 1 J 6/69 K   1.00F   1.00    0.00    0.00    0.00 2   58.0967032          0.000
   1131.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.655546900D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.926802500D+04-4.117993200D+01
KHF2(a)
 1 J 6/71 K   1.00H   1.00F   2.00    0.00    0.00 1   78.1030464    -931297.731
    300.000    469.8507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-9.129849800D+00 8.661888900D-02 4.390441200D-05
-6.686759900D-07 8.045416300D-10              -1.125825900D+05 4.108280000D+01
KHF2(b)
 1 J 6/71 K   1.00H   1.00F   2.00    0.00    0.00 2   78.1030464          0.000
    469.850    511.9507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.205737800D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.145712600D+05-5.417014000D+01
KHF2(L)
 2 J 6/71 K   1.00H   1.00F   2.00    0.00    0.00 3   78.1030464          0.000
    511.950   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.258073700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.140430900D+05-5.587991500D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.258073700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.140430900D+05-5.587991500D+01
KOH(a)          Alpha,beta. JPCRD v26 n4,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 1   56.1056400    -423400.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12600.000
-4.380064620D+05 1.125472885D+04-1.023623342D+02 4.375630440D-01-5.920346390D-04
 0.000000000D+00 0.000000000D+00              -1.002155756D+05 5.241308280D+02
KOH(b)          Beta.      JPCRD v26 n4,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 2   56.1056400    -423400.000
    298.150    517.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12600.000
-2.814357070D+03 0.000000000D+00 6.478313214D+00 6.183767895D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.313882160D+04-2.899826328D+01
KOH(c)          Gamma.     JPCRD v26 n4,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 3   56.1056400    -423400.000
    517.000    679.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12600.000
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.325857830D+04-4.413346659D+01
KOH(L)          Liquid.    JPCRD v26 n4,1997 p1031.
 1 g 8/97 K   1.00O   1.00H   1.00    0.00    0.00 4   56.1056400    -423400.000
    679.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12600.000
 0.000000000D+00 0.000000000D+00 1.046363526D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.288008340D+04-4.822385687D+01
KO2(s)
 2 J 6/71 K   1.00O   2.00    0.00    0.00    0.00 1   71.0971000    -284525.340
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.877548700D+00 3.015703100D-02-5.118225100D-05
 4.163387200D-08-1.307295600D-11              -3.634072700D+04-1.441903200D+01
   1000.000   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.049454500D+01 6.885898800D-02-8.140230700D-05
 4.294769200D-08-8.496583200D-12              -3.248998900D+04 5.968591300D+01
K2CO3(s)
 2 J 3/66 K   2.00C   1.00O   3.00    0.00    0.00 1  138.2055000   -1150194.168
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.439863200D+00 1.883625600D-02-4.682748300D-07
-1.051961000D-08 6.431841200D-12              -1.416674400D+05-3.489442400D+01
   1000.000   1174.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.282434100D+01-1.358099300D-02 8.740989000D-06
 1.149442500D-08-6.758814900D-12              -1.457784400D+05-1.104866500D+02
K2CO3(L)
 1 J 3/66 K   2.00C   1.00O   3.00    0.00    0.00 2  138.2055000          0.000
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   1174.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.516146900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.474013800D+05-1.311073000D+02
K2O(s)
 2 J 6/63 K   2.00O   1.00    0.00    0.00    0.00 1   94.1960000    -363171.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.430398720D-01 6.206377050D-02-1.362310730D-04
 1.363769720D-07-4.901638600D-11                -4.561258620D+04-4.759034700D+00
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.187026400D+00 9.114923650D-03-4.180668800D-06
 1.798982670D-09-2.839412510D-13                -4.600094260D+04-3.174498020D+01
K2O2(s)
 2 J 9/63 K   2.00O   2.00    0.00    0.00    0.00 1  110.1954000    -495804.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.826742080D+00 1.326212640D-02-1.114395780D-05
 1.095885630D-08-4.241016050D-12                -6.277352540D+04-4.025143210D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.048162990D+01 6.908618070D-03 4.865670380D-07
-2.549027230D-10 4.083861860D-14                -6.318143180D+04-4.847729020D+01
K2S(1)
 2 J 3/78 K   2.00S   1.00    0.00    0.00    0.00 1  110.2626000    -376553.662
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.136443100D+01-1.881066300D-01 5.600572700D-04
-6.970355500D-07 3.124909400D-10                -4.999740600D+04-1.281045500D+02
   1000.000   1050.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-7.484933700D+01 9.361979600D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.721793900D+03 4.496739300D+02
K2S(2)
 1 J 3/78 K   2.00S   1.00    0.00    0.00    0.00 2  110.2626000           0.000
   1050.000   1100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.564281600D+02-1.266444400D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.311441900D+05-9.279427500D+02
K2S(3)
 1 J 3/78 K   2.00S   1.00    0.00    0.00    0.00 3  110.2626000           0.000
   1100.000   1221.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.711986700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.452495300D+04-9.166651100D+01
K2S(L)
 1 J 3/78 K   2.00S   1.00    0.00    0.00    0.00 4  110.2626000           0.000
   1221.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.214292700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.652034900D+04-5.471604300D+01
K2SO4(a)
 1 J 6/78 K   2.00S   1.00O   4.00    0.00    0.00 1  174.2602000   -1437753.459
    300.000    857.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.702652600D+00 8.470971400D-02-1.763257300D-04
 1.928280300D-07-7.647089000D-11                -1.759808700D+05-7.563195100D+00
K2SO4(b)
 2 J 6/78 K   2.00S   1.00O   4.00    0.00    0.00 2  174.2602000           0.000
    857.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.380717700D+01 9.673059000D-03 4.565855100D-08
 0.000000000D+00 0.000000000D+00                -1.758532600D+05-5.844129600D+01
   1000.000   1342.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.901986600D+02 1.056963100D+00-1.347529900D-03
 7.676657600D-07-1.633744000D-10                -1.055421400D+05 1.453009400D+03
K2SO4(L)
 1 J 6/78 K   2.00S   1.00O   4.00    0.00    0.00 3  174.2602000           0.000
   1342.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.423049900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.769551900D+05-1.174022200D+02
Li(cr)          Lithium Crystal. Gurvich 1982,vIV pt 1 p245;pt 2 p286.
 2 tpis82 LI  1.00    0.00    0.00    0.00    0.00 1    6.9410000           0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4632.000
-9.860652310D+03 0.000000000D+00 2.304323850D+00 2.671663720D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.388536120D+02-1.047881690D+01
    298.150    453.6907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4632.000
 7.238825070D+04 0.000000000D+00 1.570314230D-01 6.770404150D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.049497340D+02 9.961764480D-01
Li(L)           Lithium Liquid. Gurvich 1982,vIV pt 1 p245;pt 2 p286.
 1 tpis82 LI  1.00    0.00    0.00    0.00    0.00 2    6.9410000           0.000
    453.690   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4632.000
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 2.465569230D+04 0.000000000D+00 3.755723430D+00-6.332303410D-04 3.160739480D-07
 0.000000000D+00 0.000000000D+00              -7.299116690D+02-1.701274650D+01
LiALO2(s)
 2 J12/79 LI  1.00AL  1.00O   2.00    0.00    0.00 1   65.9213380   -1188677.129
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00-5.284115600D+00 7.845258700D-02-1.454157800D-04
 1.246295800D-07-4.011370500D-11              -1.438183100D+05 1.857673300D+01
   1000.000   1973.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.544089400D+00 6.488679100D-03-4.086396900D-06
 1.547146600D-09-2.249503800D-13              -1.459815000D+05-4.459061800D+01
LiALO2(L)
 1 J12/79 LI  1.00AL  1.00O   2.00    0.00    0.00 2   65.9213380         0.000
   1973.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.509667900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.416583900D+05-8.099376700D+01
LiCL(s)
 1 J 6/62 LI  1.00CL  1.00    0.00    0.00    0.00 1   42.3937000    -408254.131
    300.000    883.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.109524500D+00 8.198100300D-03-1.154187400D-05
 1.058538600D-08-3.645702200D-12              -5.060826600D+04-1.829889400D+01
LiCL(L)
 2 J 6/62 LI  1.00CL  1.00    0.00    0.00    0.00 2   42.3937000         0.000
    883.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.038302800D+01-4.717969900D-03-1.613831700D-06
 8.080717400D-09-4.445949300D-12              -5.053912000D+04-4.992196000D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.214947700D+00 5.639136100D-04-1.735033100D-06
 7.659500800D-10-1.237847700D-13              -5.000732200D+04-3.880896100D+01
LiF(s)
 2 J12/68 LI  1.00F   1.00    0.00    0.00    0.00 1   25.9394032    -616931.953
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.769432500D+00 1.750522400D-02-2.803875100D-05
 2.289338500D-08-6.963365800D-12              -7.529927800D+04-9.947805700D+00
   1000.000   1121.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.540573800D+00-1.342108000D-04 1.782560600D-06
 8.899644400D-10-9.129665400D-13              -7.590036500D+04-2.744727600D+01
LiF(L)
 1 J12/68 LI  1.00F   1.00    0.00    0.00    0.00 2   25.9394032         0.000
   1121.300   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.719540100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.430434700D+04-3.881548700D+01
LiH(s)
 1 J 9/67 LI  1.00H   1.00    0.00    0.00    0.00 1    7.9489400     -90620.411
    300.000    961.8007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.861181200D-01 1.212795700D-02-8.690033600D-06
 5.631155500D-09-1.269348300D-12              -1.148699100D+04-3.065457500D+00
LiH(L)
 2 J 9/67 LI  1.00H   1.00    0.00    0.00    0.00 2    7.9489400         0.000
    961.800   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.498119100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.158182600D+04-4.004727800D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.498119100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.158182600D+04-4.004727800D+01
LiOH(cr)         JPCRD v25 n4,1996 p1211.
 1 g12/96 LI  1.00O   1.00H   1.00    0.00    0.00 1   23.9483400    -487500.000
    200.000    746.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7414.000
-1.219595668D+06 2.088315124D+04-1.463475482D+02 5.611591230D-01-1.084379712D-03
 1.071789730D-06-4.218923760D-10              -1.553534699D+05 7.744129160D+02
LiOH(L)          JPCRD v25 n4,1996 p1211.
 1 g12/96 LI  1.00O   1.00H   1.00    0.00    0.00 2   23.9483400    -487500.000
    746.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        7414.000
 0.000000000D+00 0.000000000D+00 1.049971676D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.050280710D+04-5.407387971D+01
Li2O(s)
 2 J 3/64 LI  2.00O   1.00    0.00    0.00    0.00 1   29.8814000    -598702.840
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00-3.172723900D-01 3.614935600D-02-5.545592100D-05
 4.179643700D-08-1.180404800D-11              -7.310619600D+04-2.288833000D+00
   1000.000   1843.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.277477600D+00 7.852167200D-03-5.222509000D-07
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-1.786442600D-09 5.396103500D-13              -7.339627800D+04-2.176549700D+01
Li2O(L)
 1 J 3/64 LI  2.00O   1.00    0.00    0.00    0.00 2   29.8814000         0.000
   1843.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.207693100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.133792100D+04-6.517497400D+01
Li2SO4(a)
 1 J12/78 LI  2.00S   1.00O   4.00    0.00    0.00 1  109.9456000   -1436366.997
    200.000    848.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-4.138735970D+00 1.069405680D-01-2.093460520D-04
 2.128928220D-07-8.016251060D-11              -1.748067760D+05 1.298357730D+01
Li2SO4(b)
 2 J12/78 LI  2.00S   1.00O   4.00    0.00    0.00 2  109.9456000   -1436366.997
    848.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.579548120D+01-2.846250520D-04 1.533011290D-07
 0.000000000D+00 0.000000000D+00              -1.803084450D+05-1.363121680D+02
   1000.000   1132.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.610265130D+01-8.293047280D-04 3.908107350D-07
 0.000000000D+00 0.000000000D+00              -1.804224450D+05-1.380080990D+02
Li2SO4(L)
 1 J12/78 LI  2.00S   1.00O   4.00    0.00    0.00 3  109.9456000   -1436366.997
   1132.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.465791320D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.780977980D+05-1.276261580D+02
Li3N(s)
 2 J 3/78 LI  3.00N   1.00    0.00    0.00    0.00 1   34.8297400    -164544.314
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.922555800D+00 2.859870200D-02-3.533694700D-05
 3.186198500D-08-1.109350100D-11              -2.167802900D+04-1.633105700D+01
   1000.000   1300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.442250300D+00 1.347773700D-02-1.942232200D-06
-2.496010900D-11 0.000000000D+00              -2.201577600D+04-2.745727500D+01
Mg(cr)          Hexagon. JPCRD 1993 v22 n1 p1.
 2 srd 93 MG  1.00    0.00    0.00    0.00    0.00 1   24.3050000         0.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4979.161
-5.412225134D+03 0.000000000D+00 1.458173723D+00 1.330204666D-02-4.098858502D-05
 4.754339101D-08 0.000000000D+00              -7.759472010D+02-6.989702348D+00
    298.150    923.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4979.161
-2.860060304D+04 0.000000000D+00 3.398877384D+00-7.243962663D-04 1.405254188D-06
 0.000000000D+00 0.000000000D+00              -1.089519906D+03-1.545973664D+01
Mg(L)           Liquid. JPCRD 1993 v22 n1 p1.
 1 srd 93 MG  1.00    0.00    0.00    0.00    0.00 2   24.3050000         0.000
    923.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4979.161
 0.000000000D+00 0.000000000D+00 4.125318269D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.589919480D+02-1.937828582D+01
MgAL2O4(s)
 2 J12/79 MG  1.00AL  2.00O   4.00    0.00    0.00 1  142.2656760   -2299119.533
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-6.391262500D+00 1.171886000D-01-2.132517800D-04
 1.827740500D-07-5.883199100D-11              -2.782714100D+05 2.013270100D+01
   1000.000   2408.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.469767900D+01 9.330479700D-03-3.552259800D-06
 1.155053000D-09-1.433453100D-13              -2.816641100D+05-7.666868500D+01
MgAL2O4(L)
 1 J12/79 MG  1.00AL  2.00O   4.00    0.00    0.00 2  142.2656760         0.000
   2408.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.641918800D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.688353600D+05-1.419858100D+02
MgBr2(cr)       Hexagonal. TPIS 1996 pt1 p418 pt2 p332.
 1 tpis96 MG  1.00BR  2.00    0.00    0.00    0.00 1  184.1130000    -526000.000
    298.150    984.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15500.499
-6.657036915D+04 0.000000000D+00 9.124771033D+00 1.443260036D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.627087500D+04-3.872222733D+01
MgBr2(L)        Liquid. TPIS 1996 pt1 p418 pt2 p332.
 1 tpis96 MG  1.00BR  2.00    0.00    0.00    0.00 2  184.1130000    -526000.000
    984.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       15500.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.363378060D+04-5.246637684D+01
MgCO3(cr)       Hexagonal. TPIS 1996 pt1 p429 pt2 p341.
 2 tpis96 MG  1.00C   1.00O   3.00    0.00    0.00 1   84.3139000   -1096000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11630.499
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-5.649471920D+06 1.059809340D+05-8.095953810D+02 3.267992680D+00-7.111639940D-03
 8.088247340D-06-3.758639920D-09              -6.098528470D+05 4.221968000D+03
   500.000   1263.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11630.499
-1.743337852D+05 0.000000000D+00 8.820122894D+00 7.696184141D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.353742560D+05-4.570039759D+01
MgCO3(L)        Liquid. TPIS 1996 pt1 p429 pt2 p341.
 1 tpis96 MG  1.00C   1.00O   3.00    0.00    0.00 3   84.3139000   -1096000.000
   1263.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11630.499
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.336474914D+05-9.615384273D+01
MgCL2(cr)       Hexagonal. TPIS 1996 pt1 p413 pt2 p329.
 2 tpis96 MG  1.00CL  2.00    0.00    0.00    0.00 1   95.2104000    -644300.000
   200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13770.499
 3.151271437D+05-4.986561670D+03 3.407490430D+01-6.013327030D-02 7.256223640D-05
-2.984411528D-08-5.064069590D-12              -5.608909370D+04-1.833415814D+02
   500.000    987.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13770.499
-7.745495525D+04 0.000000000D+00 9.099153167D+00 1.199709905D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.051706960D+04-4.185795845D+01
MgCL2(L)        Liquid. TPIS 1996 pt1 p413 pt2 p329.
 1 tpis96 MG  1.00CL  2.00    0.00    0.00    0.00 3   95.2104000    -644300.000
   987.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13770.499
 7.120082843D+05 0.000000000D+00 1.060122605D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.543168500D+04-4.537295861D+01
MgF2(cr)        Tetragonal. TPIS 1996 pt1 p410 pt2 p326.
 2 tpis96 MG  1.00F   2.00    0.00    0.00    0.00 1   62.3018064   -1124200.000
   200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9920.499
-8.758857470D+06 1.630690293D+05-1.234784473D+03 4.913114430D+00-1.064398199D-02
 1.204196054D-05-5.572295890D-09              -8.710379520D+05 6.452721700D+03
   500.000   1536.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9920.499
-1.863609521D+05 0.000000000D+00 9.358338615D+00 4.871002621D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.386463039D+05-4.763420955D+01
MgF2(L)         Liquid. TPIS 1996 pt1 p410 pt2 p326.
 1 tpis96 MG  1.00F   2.00    0.00    0.00    0.00 3   62.3018064   -1124200.000
  1536.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9920.499
 0.000000000D+00 0.000000000D+00 1.140175428D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.340531621D+05-5.725828106D+01
MgH2(b)         Tetragonal. TPIS 1996 pt1 p402 pt2 p321.
 1 tpis96 MG  1.00H   2.00    0.00    0.00    0.00 1   26.3208800    -75700.000
   200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5310.000
 4.034912200D+06-6.115400800D+04 3.537084270D+02-9.554057160D-01 1.260522797D-03
-6.389211330D-07 0.000000000D+00               2.799920215D+05-1.959491159D+03
MgH2(L)         Liquid.TPIS 1996 pt1 p402 pt2 p321.
 1 tpis96 MG  1.00H   2.00    0.00    0.00    0.00 2   26.3208800    -75700.000
   600.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5310.000
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.135051728D+04-4.777194561D+01
MgI2(cr)        Hexagonal. TPIS 1996 pt1 p422 pt2 p335.
 1 tpis96 MG  1.00I   2.00    0.00    0.00    0.00 1  278.1139400    -370000.000
   298.150    906.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17000.499
 0.000000000D+00 0.000000000D+00 8.291528905D+00 2.232723275D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.707187430D+04-3.179107057D+01
MgI2(L)         Liquid. TPIS 1996 pt1 p422 pt2 p335.
 1 tpis96 MG  1.00I   2.00    0.00    0.00    0.00 2  278.1139400    -370000.000
   906.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17000.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.641294920D+04-5.175282479D+01
MgO(cr)         Cubic TPIS 1996 pt1 p397 pt2 p317.
 2 tpis96 MG  1.00O   1.00    0.00    0.00    0.00 1   40.3044000    -601600.000
   200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5160.499
-8.980784570D+05 1.771245421D+04-1.449325747D+02 6.397591100D-01-1.458346800D-03
 1.715467374D-06-8.183482370D-10              -1.516290864D+05 7.439009690D+02
   500.000   3100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5160.499
-1.169521716D+05 0.000000000D+00 5.510366817D+00 1.085932905D-03-4.866191754D-07
 1.253230798D-10 0.000000000D+00              -7.443482720D+04-2.911564935D+01
MgO(L)          Liquid TPIS 1996 pt1 p397 pt2 p317.
 1 tpis96 MG  1.00O   1.00    0.00    0.00    0.00 3   40.3044000    -601600.000
  3100.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5160.499
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.609370840D+04-6.076894048D+01
Mg(OH)2(cr)     Hexagonal. TPIS 1996 pt1 p405 pt2 p323.
 2 tpis96 MG  1.00O   2.00H   2.00    0.00    0.00 1   58.3196800    -924350.000
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    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11410.000
-6.401451840D+05 8.358139990D+03-3.971145400D+01 1.231927219D-01-9.647800650D-05
 0.000000000D+00 0.000000000D+00              -1.537246903D+05 2.258495398D+02
    500.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11410.000
-5.543828430D+06 3.700868610D+04-9.088623340D+01 1.431689186D-01-9.513965240D-05
 2.532586546D-08 0.000000000D+00              -3.189450890D+05 5.801638270D+02
Mg(OH)2(L)        Liquid. TPIS 1996 pt1 p405 pt2 p323.
 1 tpis96 MG  1.00O   2.00H   2.00    0.00    0.00 2   58.3196800    -924350.000
   1100.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11410.000
-3.037581289D+05 0.000000000D+00 1.203462381D+01 2.202655358D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.158775486D+05-6.333852645D+01
MgS(cr)           Cubic. TPIS 1996 pt1 p424 pt2 p337.
 2 tpis96 MG  1.00S   1.00    0.00    0.00    0.00 1   56.3710000    -348000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8330.499
 1.862529340D+06-3.536941040D+04 2.721839670D+02-1.042907730D+00 2.246733361D-03
-2.528313530D-06 1.164923631D-09               1.157121957D+05-1.421776433D+03
    500.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8330.499
-2.774667419D+04 0.000000000D+00 5.477652922D+00 1.053219011D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.362757840D+04-2.562621459D+01
MgS(L)            Liquid. TPIS 1996 pt1 p424 pt2 p337.
 1 tpis96 MG  1.00S   1.00    0.00    0.00    0.00 3   56.3710000    -348000.000
   2500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8330.499
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.919942750D+04-4.015043492D+01
MgSO4(II)         CrII,rhombic. TPIS 1996 pt1 p426 pt2 p339.
 2 tpis96 MG  1.00S   1.00O   4.00    0.00    0.00 1  120.3686000   -1288800.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
 7.038799190D+06-1.283866938D+05 9.464955820D+02-3.562117130D+00 7.535844540D-03
-8.351428640D-06 3.800035070D-09               4.243566150D+05-4.979377480D+03
    500.000   1283.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
-1.403690656D+05 0.000000000D+00 1.024474082D+01 1.053279147D-02-2.384385851D-06
 0.000000000D+00 0.000000000D+00              -1.589785092D+05-5.117735953D+01
MgSO4(I)          CrI,rhombic. TPIS 1996 pt1 p426 pt2 p339.
 1 tpis96 MG  1.00S   1.00O   4.00    0.00    0.00 3  120.3686000   -1288800.000
   1283.000   1410.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.622917080D+05-9.940197517D+01
MgSO4(L)          Liquid. TPIS 1996 pt1 p426 pt2 p339.
 1 tpis96 MG  1.00S   1.00O   4.00    0.00    0.00 4  120.3686000   -1288800.000
   1410.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15400.499
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.605357417D+05-9.815660894D+01
MgSiO3(I)
 1 J12/67 MG  1.00SI  1.00O   3.00    0.00    0.00 1  100.3887000   -1548931.619
    300.000    903.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.337777900D+00 4.445322200D-02-6.597375300D-05
 4.741425700D-08-1.233109800D-11              -1.881722600D+05-1.017893600D+01
MgSiO3(II)
 2 J12/67 MG  1.00SI  1.00O   3.00    0.00    0.00 2  100.3887000         0.000
    903.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.447388600D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.916217200D+05-7.665946400D+01
   1000.000   1258.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.447388600D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.916217200D+05-7.665946400D+01
MgSiO3(III)
 1 J12/67 MG  1.00SI  1.00O   3.00    0.00    0.00 3  100.3887000         0.000
   1258.000   1850.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.472550100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.917419900D+05-7.829929800D+01
MgSiO3(L)
 1 J12/67 MG  1.00SI  1.00O   3.00    0.00    0.00 4  100.3887000         0.000
   1850.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.761303100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.880257900D+05-9.512573100D+01
MgTiO3(s)
 2 J 6/67 MG  1.00TI  1.00O   3.00    0.00    0.00 1  120.1702000   -1572593.459
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.577774300D-01 6.201839700D-02-1.048059600D-04
 8.494092500D-08-2.636729500D-11              -1.910773800D+05-4.661653500D+00
   1000.000   1953.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
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 0.000000000D+00 0.000000000D+00 1.028822400D+01 1.034373000D-02-7.401217900D-06
 2.792882400D-09-3.953244800D-13              -1.928116800D+05-5.295808800D+01
MgTiO3(L)
 1 J 6/67 MG  1.00TI  1.00O   3.00    0.00    0.00 2  120.1702000         0.000
   1953.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.962594900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.909181200D+05-1.065620400D+02
MgTi2O5(s)
 2 J 6/67 MG  1.00TI  2.00O   5.00    0.00    0.00 1  200.0360000   -2509409.513
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.271631100D+00 9.266379400D-02-1.636950200D-04
 1.390337300D-07-4.451323200D-11              -3.051161300D+05-1.242210200D+01
   1000.000   1963.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.677660800D+01 1.223779100D-02-6.301316000D-06
 2.401948800D-09-3.541293000D-13              -3.075465500D+05-8.329339000D+01
MgTi2O5(L)
 1 J 6/67 MG  1.00TI  2.00O   5.00    0.00    0.00 2  200.0360000         0.000
   1963.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 3.140151900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.041000100D+05-1.685864900D+02
Mg2SiO4(s)
 2 J12/67 MG  2.00SI  1.00O   4.00    0.00    0.00 1  140.6931000   -2176951.170
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.342898200D+00 6.686658800D-02-9.644562500D-05
 6.642396000D-08-1.718399000D-11              -2.644690100D+05-1.239916200D+01
   1000.000   2171.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.575267900D+01 6.800465000D-03-1.620395100D-06
 7.736811200D-12 6.333757300D-14              -2.672995500D+05-8.145799200D+01
Mg2SiO4(L)
 1 J12/67 MG  2.00SI  1.00O   4.00    0.00    0.00 2  140.6931000         0.000
   2171.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.465824400D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.669254900D+05-1.346151000D+02
Mg2TiO4(s)
 2 J 6/67 MG  2.00TI  1.00O   4.00    0.00    0.00 1  160.4746000   -2164430.666
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-5.044115600D-02 8.808642400D-02-1.568378900D-04
 1.340184700D-07-4.312378700D-11              -2.630786500D+05-6.253750700D+00
   1000.000   2013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.477257700D+01 1.082414700D-02-4.990756000D-06
 1.740794400D-09-2.539819500D-13              -2.653907800D+05-7.393371000D+01
Mg2TiO4(L)
 1 J 6/67 MG  2.00TI  1.00O   4.00    0.00    0.00 2  160.4746000         0.000
   2013.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.747632900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.615355900D+05-1.474583700D+02
Mg3N2(cr)        Cubic. TPIS 1996 pt1 p427 pt2 p340.
 1 tpis96 MG  3.00N   2.00    0.00    0.00    0.00 1  100.9284800    -461300.000
    298.150   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10500.499
-3.313123684D+05 0.000000000D+00 1.448912804D+01 1.035659347D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.095851350D+04-7.450243529D+01
Mn(a)           Manganese Alpha crystal.  JANAF Sep.1967.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 1   54.9380490         0.000
    200.000    980.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4994.000
-1.984724750D+04 1.808814270D+02 1.038289720D+00 8.813332260D-03-1.298046010D-05
 1.118858770D-08-3.673641390D-12              -1.704143090D+03-3.713160510D+00
Mn(b)           Manganese Beta crystal.  JANAF Sep.1967.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 2   54.9380490         0.000
    980.000   1361.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4994.000
-2.067667860D+08 8.744754920D+05-1.470433420D+03 1.239522230D+00-5.189221550D-04
 8.666005810D-08 0.000000000D+00              -5.242434740D+06 9.928233970D+03
Mn(c)           Manganese Gamma crystal.  JANAF Sep.1967.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 3   54.9380490         0.000
   1361.000   1412.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4994.000
-5.539098660D+06 0.000000000D+00 1.249141100D+01-3.172628690D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.319366010D+04-7.700747410D+01
Mn(d)           Manganese Delta crystal.  JANAF Sep.1967.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 4   54.9380490         0.000
   1412.000   1519.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4994.000
-4.256308770D+06 0.000000000D+00 1.001246350D+01-1.726532590D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.000047710D+04-6.058839120D+01
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Mn(L)          Manganese Liquid.  JANAF Sep.1967.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 5   54.9380490         0.000
   1519.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4994.000
 0.000000000D+00 0.000000000D+00 5.535383320D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.393768830D+02-2.853570330D+01
Mo(cr)         Molybdenum Crystal. JANAF Mar.1978.
 3 j 3/78 MO  1.00    0.00    0.00    0.00    0.00 1   95.9400000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4585.000
-4.961689360D+04 4.280941240D+02 7.671984370D-01 5.731518340D-03-6.381641320D-06
 3.708192530D-09-7.917347440D-13               -3.039584650D+03-1.230467510D+00
   1000.000   2200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4585.000
-3.614786560D+06 1.473478790D+04-2.134702700D+01 2.116823010D-02-9.781092030D-06
 2.493890290D-09-2.419922290D-13               -8.970924690D+04 1.505836440D+02
   2200.000   2896.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4585.000
 3.271666300D+09-1.774787110D+06-4.389955150D+03 5.649396210D+00-2.680925240D-03
 5.840314270D-07-4.893484920D-11                1.773917680D+07 2.560041870D+04
Mo(L)          Molybdenum Liquid. JANAF Mar.1978.
 1 j 3/78 MO  1.00    0.00    0.00    0.00    0.00 2   95.9400000         0.000
   2896.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4585.000
 0.000000000D+00 0.000000000D+00 4.528949990D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.022318520D+03-2.280791020D+01
NH4CL(a)
 1 BAR 73 N   1.00H   4.00CL  1.00    0.00    0.00 1   53.4912000    -314556.854
    298.150    458.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.674938300D+00 1.927342500D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.008275100D+04-2.095913300D+01
NH4CL(b)
 1 BAR 73 N   1.00H   4.00CL  1.00    0.00    0.00 2   53.4912000    -314556.854
    458.000    793.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.166685000D+00 1.343604900D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.876269300D+04-1.413440200D+01
NH4F(cr)        Ammonium Fluoride Hexagonal Crystal. TPIS,1989.
 2 tpis89 N   1.00H   4.00F   1.00    0.00    0.00 1   37.0369032    -467560.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11108.000
-2.246351510D+06 5.410877010D+04-5.507050000D+02 3.075888060D+00-9.598095080D-03
 1.619888730D-05-1.149746540D-08               -2.863677530D+05 2.704329200D+03
    298.150    511.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11108.000
 0.000000000D+00 0.000000000D+00 1.563531700D+00 2.108482640D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -5.763754000D+04-6.538862040D+00
NH4F(L)         Ammonium Fluoride Liquid. TPIS,1989.
 1 tpis89 N   1.00H   4.00F   1.00    0.00    0.00 3   37.0369032    -467560.000
    511.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11108.000
 0.000000000D+00 0.000000000D+00 1.359069870D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -5.951515380D+04-6.780477120D+01
Na(cr)         Sodium Cubic Crystal.  CODATA 1989, p254.
 1 coda89 NA  1.00    0.00    0.00    0.00    0.00 1   22.9897700         0.000
    200.000    371.0107 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6460.000
-3.584457960D+04 0.000000000D+00 6.479414670D+00-1.898697330D-02 3.352387080D-05
 0.000000000D+00 0.000000000D+00               -1.504319740D+03-2.677783030D+01
Na(L)          Sodium Liquid.  CODATA 1989, p254.
 1 coda89 NA  1.00    0.00    0.00    0.00    0.00 2   22.9897700         0.000
    371.010   2300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6460.000
 2.694838720D+04-2.319013910D+02 5.162438950D+00-3.058576020D-03 1.696410610D-06
-1.519641960D-10 1.962870170D-14               2.842187620D+02-2.225766060D+01
NaALO2(a)
 1 J 3/63 NA  1.00AL  1.00O   2.00    0.00    0.00 1   81.9701080   -1133223.447
    300.000    740.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-8.050478000D-01 5.843496800D-02-1.188441500D-04
 1.197004200D-07-4.622479300D-11               -1.378166500D+05-5.333528200D-02
NaALO2(b)
 2 J 3/63 NA  1.00AL  1.00O   2.00    0.00    0.00 2   81.9701080         0.000
    740.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.054234300D+01 8.848390700D-04 1.390676300D-06
-5.139139300D-10 0.000000000D+00               -1.395806000D+05-5.237136200D+01
   1000.000   3000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.196621500D+01-2.281727700D-03 3.771374100D-06
-1.293267000D-09 1.413502200D-13               -1.400481800D+05-6.000645500D+01
NaBr(s)
 2 J 9/64 NA  1.00BR  1.00    0.00    0.00    0.00 1  102.8937700    -361417.497
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.876646100D+00 6.831892800D-03-1.064116300D-05
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 9.161392800D-09-2.881629700D-12              -4.514864400D+04-1.898254500D+01
   1000.000   1020.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.624644800D+00 1.238298300D-04 4.099027600D-07
 2.068365100D-10-1.807648500D-14              -4.556037200D+04-2.760580000D+01
NaBr(L)
 1 J 9/64 NA  1.00BR  1.00    0.00    0.00    0.00 2  102.8937700         0.000
   1020.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.498119100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.304977000D+04-3.017045100D+01
NaCN(s)
 1 J 3/66 NA  1.00C   1.00N   1.00    0.00    0.00 1   49.0072100    -90679.248
    300.000    835.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.996773200D+00 1.915455000D-03-5.342159100D-06
 6.809164200D-09-3.141491100D-12              -1.334029400D+04-3.170393300D+01
NaCN(L)
 2 J 3/66 NA  1.00C   1.00N   1.00    0.00    0.00 2   49.0072100         0.000
    835.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.561360000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.338640700D+04-4.028730900D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.561360000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.338640700D+04-4.028730900D+01
NaCL(s)
 2 J 9/64 NA  1.00CL  1.00    0.00    0.00    0.00 1   58.4424700   -411131.194
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.024077800D+00 5.194906600D-03-7.283373000D-06
 6.067197900D-09-1.201342400D-12              -5.112333500D+04-2.122720100D+01
   1000.000   1073.8007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.213492700D+00 1.585990200D-03 5.048638300D-06
 2.602054900D-09-3.648709600D-12              -4.926320300D+04-2.602566000D+00
NaCL(L)
 1 J 9/64 NA  1.00CL  1.00    0.00    0.00    0.00 2   58.4424700         0.000
   1073.800   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.235848800D+01-6.307120100D-03 3.200472300D-06
-6.771736200D-10 5.101561200D-14              -5.142326500D+04-6.058553000D+01
NaF(s)
 2 J12/68 NA  1.00F   1.00    0.00    0.00    0.00 1   41.9881732   -575391.674
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.697755200D+00 1.052057200D-02-1.723565600D-05
 1.412591100D-08-3.951452900D-12              -7.064718300D+04-1.739363300D+01
   1000.000   1269.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.834202600D+00-9.483918000D-04-5.484398600D-06
 8.684302200D-09-2.928586000D-12              -7.181040500D+04-3.881571000D+01
NaF(L)
 1 J12/68 NA  1.00F   1.00    0.00    0.00    0.00 2   41.9881732         0.000
   1269.000   3500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.096326100D+01-3.206845900D-03 1.161166200D-06
-1.629929700D-10 5.245614100D-15              -7.067394300D+04-5.637569500D+01
NaI(s)
 1 J 9/63 NA  1.00I   1.00    0.00    0.00    0.00 1  149.8942400   -287861.511
    300.000    933.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.499598400D+00 3.566805300D-03-3.996563000D-06
 3.184107300D-09-9.530872200D-13              -3.639035600D+04-2.039925100D+01
NaI(L)
 2 J 9/63 NA  1.00I   1.00    0.00    0.00    0.00 2  149.8942400         0.000
    933.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.800056800D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.475956800D+04-3.081888100D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.800056800D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.475956800D+04-3.081888100D+01
NaOH(a)          alpha. JPCRD 1996 v25 n4 p1211.
 2 g 5/99 NA  1.00O   1.00H   1.00    0.00    0.00 1   39.9971100   -425800.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      10490.000
 2.008329119D+04-7.714677160D+02 8.694171090D+00 3.850883340D-03-3.610498540D-06
 0.000000000D+00 0.000000000D+00              -4.948023450D+04-4.524899570D+01
    298.150    514.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      10490.000
 1.048215710D+06 0.000000000D+00-9.592892425D+01 6.189564989D-01-1.367212259D-03
 1.067453163D-06 0.000000000D+00              -3.663541040D+04 4.270051072D+02
NaOH(b)          beta.  JPCRD 1996 v25 n4 p1211.
 1 g 5/99 NA  1.00O   1.00H   1.00    0.00    0.00 3   39.9971100   -425800.000
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   514.000    568.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10490.000
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.442558950D+04-4.799292559D+01
NaOH(c)          gamma. JPCRD 1996 v25 n4 p1211.
 1 g 5/99 NA  1.00O   1.00H   1.00    0.00    0.00 4   39.9971100    -425800.000
   568.000    594.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10490.000
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.407054750D+04-5.122288687D+01
NaOH(L)          Liquid.JPCRD 1996 v25 n4 p1211.
 2 g 5/99 NA  1.00O   1.00H   1.00    0.00    0.00 5   39.9971100    -425800.000
   594.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10490.000
 0.000000000D+00 0.000000000D+00 1.077790513D+01-7.111663826D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.343827480D+04-5.228806116D+01
  1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10490.000
 0.000000000D+00 0.000000000D+00 1.006673875D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.308269160D+04-4.808666421D+01
NaO2(s)
 2 J 6/63 NA  1.00O   2.00    0.00    0.00    0.00 1   54.9885700    -260669.371
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 7.279888200D+00 4.416072100D-03 1.241392100D-06
-1.292117100D-09 4.825947900D-13                -3.372656100D+04-2.889980700D+01
  1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 6.675317700D+00 6.423451300D-03-1.543777300D-06
 6.835777400D-10-1.107392200D-13                -3.357254600D+04-2.584860800D+01
Na2CO3(I)
 1 J 3/66 NA  2.00C   1.00O   3.00    0.00    0.00 1  105.9884400   -1130792.209
   300.000    723.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 6.783565900D+00 3.882970100D-02-9.826245500D-05
 1.654308400D-07-8.329451500D-11                -1.391701000D+05-3.046329300D+01
Na2CO3(II)
 2 J 3/66 NA  2.00C   1.00O   3.00    0.00    0.00 2  105.9884400          0.000
   723.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 1.184834100D+01-3.513898600D-03 2.061556900D-05
-7.396517500D-09 0.000000000D+00                -1.381418700D+05-4.806436800D+01
  1000.000   1123.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 8.281775500D+00 1.127538900D-02 1.996329400D-06
 0.000000000D+00 0.000000000D+00                -1.376126600D+05-3.137258000D+01
Na2CO3(L)
 1 J 3/66 NA  2.00C   1.00O   3.00    0.00    0.00 3  105.9884400          0.000
  1123.150   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 2.279629500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.422921800D+05-1.162212100D+02
Na2O(c)
 2 J 6/68 NA  2.00O   1.00    0.00    0.00    0.00 1   61.9789400    -417992.144
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 5.265458300D+00 1.111687200D-02-6.387538200D-07
-9.699320700D-09 5.372007100D-12                -5.231434500D+04-2.418702400D+01
  1000.000   1243.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 2.416895600D+01-2.527974400D-02-4.739065800D-06
 3.183638700D-08-1.457026500D-11                -5.804823600D+04-1.251806500D+02
Na2O(a)
 1 J 6/68 NA  2.00O   1.00    0.00    0.00    0.00 2   61.9789400          0.000
  1243.200   1405.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00-1.490659000D+02 2.279903800D-01 3.839126800D-05
-1.709991900D-07 6.139592600D-11                1.161479500D+04 8.468926800D+02
Na2O(L)
 1 J 6/68 NA  2.00O   1.00    0.00    0.00    0.00 3   61.9789400          0.000
  1405.200   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 1.258073700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -4.859485700D+04-6.066154900D+01
Na2O2(a)
 1 J 6/68 NA  2.00O   2.00    0.00    0.00    0.00 1   77.9783400    -513227.637
   300.000    785.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 4.581527800D+00 3.245591000D-02-5.115420100D-05
 4.266397900D-08-1.399163700D-11                -6.416105300D+04-2.245545300D+01
Na2O2(b)
 2 J 6/68 NA  2.00O   2.00    0.00    0.00    0.00 2   77.9783400          0.000
   785.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
 0.000000000D+00 0.000000000D+00 1.366268000D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.563257100D+04-6.684155100D+01
  1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            0.000
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 0.000000000D+00 0.000000000D+00 1.366268000D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.563257100D+04-6.684155100D+01
Na2S(1)
 2 J 3/78 NA  2.00S   1.00    0.00    0.00    0.00 1   78.0455400    -366105.021
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.707559900D+00-3.112618300D-04 5.512116100D-06
-6.043507200D-09 2.301754900D-12              -4.695037900D+04-4.383761300D+01
   1000.000   1276.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.467556000D+02-1.058511100D+00 8.117009300D-04
-1.887787800D-07 0.000000000D+00              -1.774839400D+05-2.346265900D+03
Na2S(2)
 1 J 3/78 NA  2.00S   1.00    0.00    0.00    0.00 2   78.0455400         0.000
   1276.000   1445.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-5.679354900D+05 1.680412100D+03-1.862267900D+00
 9.162058800D-04-1.688487900D-07              1.533280500D+08 2.910868700D+06
Na2S(L)
 1 J 3/78 NA  2.00S   1.00    0.00    0.00    0.00 3   78.0455400         0.000
   1445.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.107104800D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.279093000D+04-4.861588900D+01
Na2SO3(s)        Sodium Sulfite. Barin,Ihsan:1989 ptII p1002.
 1 bar 89 NA  2.00S   1.00O   3.00    0.00    0.00 1  126.0437400   -1100802.000
    298.150   1184.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.290193602D+01 5.233511440D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.364746191D+05-5.751819280D+01
Na2SO3(L)        Sodium Sulfite. Barin,Ihsan:1989 ptII p1002.
 1 bar 89 NA  2.00S   1.00O   3.00    0.00    0.00 2  126.0437400   -1100802.000
   1184.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.403382187D+05-1.123000267D+02
Na2SO4(V)
 1 J 6/78 NA  2.00S   1.00O   4.00    0.00    0.00 1  142.0431400   -1387815.996
    200.000    458.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.833931860D+00 3.082019920D-02 5.979863500D-05
-2.597790780D-07 2.478539980D-10              -1.701560750D+05-2.528864270D+01
Na2SO4(IV)
 1 J 6/78 NA  2.00S   1.00O   4.00    0.00    0.00 2  142.0431400   -1387815.996
    458.000    514.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.719677840D+00 2.188204200D-02-6.197707470D-06
 0.000000000D+00 0.000000000D+00              -1.707128190D+05-4.360633690D+01
Na2SO4(I)
 2 J 6/78 NA  2.00S   1.00O   4.00    0.00    0.00 3  142.0431400   -1387815.996
    514.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.548543890D+01 1.926137770D-02-3.322573320D-05
 3.562833020D-08-1.305772140D-11              -1.713229230D+05-7.351270150D+01
   1000.000   1157.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.611573890D+01 8.209258910D-03-2.333055470D-07
 0.000000000D+00 0.000000000D+00              -1.711291010D+05-7.469907480D+01
Na2SO4(L)
 1 J 6/78 NA  2.00S   1.00O   4.00    0.00    0.00 4  142.0431400   -1387815.996
   1157.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.369777290D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.716589120D+05-1.163584820D+02
Na3ALF6(a)
 1 J12/79 NA  3.00AL  1.00F   6.00    0.00    0.00 1  209.9412672   -3316981.881
    300.000    836.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.259295800D+00 1.556966600D-01-3.616184400D-04
 4.047908000D-07-1.650555200D-10              -4.040599300D+05-1.779854500D+01
Na3ALF6(b)
 2 J12/79 NA  3.00AL  1.00F   6.00    0.00    0.00 2  209.9412672         0.000
    836.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.659365700D+01 1.691169400D-02 1.031660000D-06
 0.000000000D+00 0.000000000D+00              -4.010868900D+05-6.491079200D+01
   1000.000   1285.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 9.554395700D+00 3.520154200D-02-1.462099400D-05
 4.402066900D-09 0.000000000D+00              -3.990755200D+05-2.821617700D+01
Na3ALF6(L)
 1 J12/79 NA  3.00AL  1.00F   6.00    0.00    0.00 3  209.9412672         0.000
   1285.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.756762300D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.129653800D+05-2.537588000D+02
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Na5AL3F14(s)
 2 J12/79 NA  5.00AL  3.00F  14.00    0.00    0.00 1  461.8711088   -7581530.319
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.372817100D+01 2.329830000D-01-4.167217200D-04
 3.537326800D-07-1.127677400D-10              -9.232558200D+05-7.391375400D+01
   1000.000   1010.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.080537600D+01 1.014901500D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.319436500D+05-2.949194800D+02
Na5AL3F14(L)
 1 J12/79 NA  5.00AL  3.00F  14.00    0.00    0.00 2  461.8711088         0.000
   1010.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.171301000D+02 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.561288400D+05-6.470530900D+02
Nb(cr)          Niobium Crystal.  JANAF, Dec. 1973.
 3 j12/73 NB  1.00    0.00    0.00    0.00    0.00 1   92.9063800         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5241.000
-4.254812210D+04 3.875297820D+02 1.184449320D+00 4.507437830D-03-5.232093820D-06
 3.513453860D-09-9.507610030D-13              -2.864449670D+03-2.442972790D+00
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5241.000
 2.525853960D+07-1.084926930D+05 1.927760810D+02-1.726112770D-01 8.664448040D-05
-2.264294570D-08 2.435282590D-12              6.467586620D+05-1.283088040D+03
   2000.000   2750.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5241.000
-1.350960570D+09 3.880052900D+06-4.560679500D+03 2.817075580D+00-9.625208980D-04
 1.726201040D-07-1.266340690D-11              -2.471700570D+07 3.232835990D+04
Nb(L)           Niobium Liquid.  JANAF, Dec. 1973.
 1 j12/73 NB  1.00    0.00    0.00    0.00    0.00 2   92.9063800         0.000
   2750.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5241.000
 0.000000000D+00 0.000000000D+00 4.025733330D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               1.427053200D+03-1.857964880D+01
NbO(s)
 2 J12/73 NB  1.00O   1.00    0.00    0.00    0.00 1  108.9057800    -419661.164
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.982126000D+00 1.021754500D-02-1.517889500D-05
 1.130846700D-08-3.138285800D-12              -5.170336900D+04-1.391859700D+01
   1000.000   2210.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.123655300D+00 8.937586000D-04 3.093084500D-07
-1.643370200D-10 2.856983500D-14              -5.211091000D+04-2.409952000D+01
NbO(L)
 1 J12/73 NB  1.00O   1.00    0.00    0.00    0.00 2  108.9057800         0.000
   2210.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.548442100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.458713800D+04-3.581734000D+01
NbOCL3(cr)       Barin 1989. JPCRD v11 1982 sup2.
 1 bar 89 NB  1.00O   1.00CL  3.00    0.00    0.00 1  215.2638800    -879500.000
    298.150    702.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
-1.822304138D+05 4.828593360D+02 1.341861113D+01 7.546458250D-03-1.198129404D-05
 9.997155720D-09-3.425554610D-12              -1.133897355D+05-6.057973360D+01
NbO2(I)
 2 J12/73 NB  1.00O   2.00    0.00    0.00    0.00 1  124.9051800    -794960.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00-1.548417920D+00 5.455364280D-02-1.206746260D-04
 1.237777700D-07-4.561548080D-11              -9.673116300D+04 3.472682150D+00
   1000.000   1090.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.289027160D+00 5.203860620D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.729724610D+04-2.489085970D+01
NbO2(II)
 1 J12/73 NB  1.00O   2.00    0.00    0.00    0.00 2  124.9051800    -794960.000
   1090.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.117141000D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.002059980D+05-5.998194410D+01
NbO2(III)
 1 J12/73 NB  1.00O   2.00    0.00    0.00    0.00 3  124.9051800    -794960.000
   1200.000   2175.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.988850820D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.878692740D+04-5.159750880D+01
NbO2(L)
 1 J12/73 NB  1.00O   2.00    0.00    0.00    0.00 4  124.9051800    -794960.000
   2175.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.132237500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.061657580D+04-5.675534620D+01
Nb2O5(s)
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 2 J12/72 NB  2.00O   5.00    0.00    0.00    0.00 1  265.8097600   -1899558.522
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 8.505348800D+00 3.440121400D-02-3.769874800D-05
 1.986372000D-08-3.961026700D-12              -2.322322900D+05-4.068492000D+01
   1000.000   1785.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.705489200D+01 4.914055800D-03 4.729464400D-07
-1.837607100D-09 5.062192200D-13              -2.342302700D+05-8.322479900D+01
Nb2O5(L)
 1 J12/72 NB  2.00O   5.00    0.00    0.00    0.00 2  265.8097600         0.000
   1785.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.913698700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.373602500D+05-1.593339600D+02
Ni(cr)          Nickel Crystal below lambda trans 631K. JANAF Dec.1976.
 2 j12/76 NI  1.00    0.00    0.00    0.00    0.00 1   58.6934000         0.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4786.000
-7.686918970D+05 1.433563570D+04-1.042476920D+02 3.925316950D-01-6.985305610D-04
 4.905008120D-07 0.000000000D+00              -6.541997360D+04 5.509928300D+02
    400.000    631.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4786.000
-3.332260450D+08 3.410969830D+06-1.389067090D+04 2.815138150D+01-2.837537990D-02
 1.138819010D-05 0.000000000D+00              -1.743282120D+07 8.148263870D+04
Ni(cr)          Nickel Crystal above lambda trans 631K. JANAF Dec.1976.
 2 j12/76 NI  1.00    0.00    0.00    0.00    0.00 2   58.6934000         0.000
    631.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4786.000
 1.047299940D+09-6.890030590D+06 1.876557690D+04-2.706863450D+01 2.182286740D-02
-9.321377810D-06 1.648170960D-09              3.813973330D+07-1.171340620D+05
   1200.000   1728.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4786.000
 1.852047680D+09-7.142958210D+06 1.137639760D+04-9.560804970D+00 4.471493020D-03
-1.101283630D-06 1.114042950D-10              4.336289880D+07-7.713008040D+04
Ni(L)           Nickel Liquid. JANAF Dec.1976.
 1 j12/76 NI  1.00    0.00    0.00    0.00    0.00 3   58.6934000         0.000
   1728.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4786.000
 0.000000000D+00 0.000000000D+00 4.679890940D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.216178080D+02-2.335476580D+01
NiS(b)
 1 J12/76 NI  1.00S   1.00    0.00    0.00    0.00 1   90.7594000    -87868.633
    300.000    652.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.515051300D+00 1.981087900D-02-4.475171300D-05
 5.355273600D-08-2.473915100D-11              -1.189727500D+04-1.229880500D+01
NiS(a)
 2 J12/76 NI  1.00S   1.00    0.00    0.00    0.00 2   90.7594000         0.000
    652.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.597785500D+00 1.627915900D-02-2.395926400D-05
 1.966524700D-08-5.999359200D-12              -1.060519200D+04-4.998841400D+00
   1000.000   1249.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00-2.168827700D+00 2.046726100D-02-1.523906800D-05
 4.524203900D-09 0.000000000D+00              -9.253973100D+03 1.601897600D+01
NiS(L)
 1 J12/76 NI  1.00S   1.00    0.00    0.00    0.00 3   90.7594000         0.000
   1249.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 9.234260800D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.105365200D+04-4.576973600D+01
NiS2(s)
 2 J 3/77 NI  1.00S   2.00    0.00    0.00    0.00 1  122.8254000    -131380.855
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 7.744934900D+00 2.535171400D-03-9.976758700D-08
 1.078295000D-10-4.191294100D-14              -1.822253900D+04-3.622438800D+01
   1000.000   1280.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 5.274264000D+00 9.087093100D-03-5.820109900D-06
 1.705008100D-09 0.000000000D+00              -1.752872500D+04-2.339221900D+01
NiS2(L)
 1 J 3/77 NI  1.00S   2.00    0.00    0.00    0.00 2  122.8254000         0.000
   1280.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.094524100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.234492500D+04-4.972062400D+01
Ni3S2(I)
 1 J12/76 NI  3.00S   2.00    0.00    0.00    0.00 1  240.2122000    -216325.162
    300.000    829.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.923830000D+00 4.044668000D-02-7.307395700D-05
 7.100707600D-08-2.622185900D-11              -2.936219600D+04-3.273505200D+01
Ni3S2(II)
 2 J12/76 NI  3.00S   2.00    0.00    0.00    0.00 2  240.2122000         0.000
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   829.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.268558500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.931347900D+04-1.116897800D+02
   1000.000   1062.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.268558500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.931347900D+04-1.116897800D+02
Ni3S2(L)
 1 J12/76 NI  3.00S   2.00    0.00    0.00    0.00 3  240.2122000         0.000
   1062.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.306803900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.734440200D+04-1.121181100D+02
Ni3S4(s)
 2 J 3/77 NI  3.00S   4.00    0.00    0.00    0.00 1  304.3442000    -301121.261
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.467119300D+01 1.727716400D-02-2.756928400D-09
 1.023385800D-11-6.298395600D-15              -4.135847900D+04-6.631293900D+01
   1000.000   1100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.467381800D+01 1.727571800D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.136000100D+04-6.632916200D+01
P(cr)           Crystal(White). TPIS 1989 v1 pt2 p326.
 1 tpis89 P   1.00    0.00    0.00    0.00    0.00 1   30.9737610         0.000
   195.400    317.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       5360.000
-5.183070130D+06 1.237702260D+05-1.223276610D+03 6.436736650D+00-1.890194970D-02
 2.947034970D-05-1.905868050D-08              -5.261975990D+05 6.058963430D+03
P(L)            Liquid. TPIS 1989 v1 pt2 p326.
 1 tpis89 P   1.00    0.00    0.00    0.00    0.00 2   30.9737610         0.000
   317.300   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       5360.000
 0.000000000D+00 0.000000000D+00 3.141496010D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.621432860D+02-1.272273010D+01
P4O10(cr)        Crystal. TPIS 1989 v1 pt1 p417; pt2 p270.
 2 tpis89 P   4.00O  10.00    0.00    0.00    0.00 1  283.8890440   -3010100.000
   100.000   298.150 3 -2.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0      34220.000
-2.910475984D+04 5.209612140D+00 7.058407940D-02 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00 0.000000000D+00-3.668178470D+05-2.310786251D+01
   298.150   699.000 3  0.0  1.0  2.0  0.0  0.0  0.0  0.0  0.0      34220.000
 5.461897334D+00 8.078166964D-02-4.072398734D-05 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00 0.000000000D+00-3.668889200D+05-2.561194012D+01
P4O10(L)         Liquid. TPIS 1989 v1 pt1 p417; pt2 p270.
 1 tpis89 P   4.00O  10.00    0.00    0.00    0.00 3  283.8890440   -3010100.000
   699.000  6000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0      34220.000
 4.450051777D+01 0.000000000D+00 0.000000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00 0.000000000D+00-3.765523910D+05-2.311704609D+02
Pb(cr)           Cubic. TPIS 1991 v2 pt1 p400 pt22 p337.
 1 tpis91 PB  1.00    0.00    0.00    0.00    0.00 1  207.2000000         0.000
   200.000    600.6507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6870.000
-6.149633710D+05 1.065711680D+04-7.129853690D+01 2.668390070D-01-5.181983860D-04
 5.238630120D-07-2.151630770D-10              -4.974048400D+04 3.855802060D+02
Pb(L)            Liquid. TPIS 1991v2 pt1 p400 pt22 p337.
 1 tpis91 PB  1.00    0.00    0.00    0.00    0.00 2  207.2000000         0.000
   600.650   3600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6870.000
-3.798179330D+04 0.000000000D+00 4.364298080D+00-1.236392760D-03 4.946773770D-07
-5.231817630D-11 0.000000000D+00              -8.887330460D+02-1.619559680D+01
PbBr2(s)         Rhombic Crystal. TPIS 1991 v2 pt1 p435;pt2 p361.
 2 tpis91 PB  1.00BR  2.00    0.00    0.00    0.00 1  367.0080000    -276700.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19230.000
 0.000000000D+00 0.000000000D+00 6.565717260D+00 1.959605210D-02-3.191530530D-05
 0.000000000D+00 0.000000000D+00              -3.582576310D+04-2.245707570D+01
   298.150    644.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19230.000
 8.046174700D+04 0.000000000D+00 6.899264060D+00 5.925905430D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.532970360D+04-2.124769270D+01
PbBr2(L)         Liquid. TPIS 1991 v2 pt1 p435;pt2 p361.
 1 tpis91 PB  1.00BR  2.00    0.00    0.00    0.00 3  367.0080000    -276700.000
   644.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19230.000
 0.000000000D+00 0.000000000D+00 1.347042700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.648036370D+04-5.695842620D+01
PbCL2(cr)        Rhombic Crystal. TPIS 1991 v2 pt1 p428;pt2 p356.
 1 tpis91 PB  1.00CL  2.00    0.00    0.00    0.00 1  278.1054000    -359400.000
   200.000    774.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      17150.000
 2.697281121D+06-4.212942350D+04 2.651641932D+02-7.891350070D-01 1.316948609D-03
-1.123561948D-06 3.854416550D-10              1.522766773D+05-1.434661776D+03
PbCL2(L)         Liquid. TPIS 1991 v2 pt1 p428;pt2 p356.
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 1 tpis91 PB  1.00CL  2.00    0.00    0.00    0.00 2  278.1054000    -359400.000
    774.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        17150.000
 0.000000000D+00 0.000000000D+00 1.335015533D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.613690180D+04-5.953419614D+01
PbF2(II)         Rhombic Crystal(II). TPIS 1991 v2 pt1 p421;pt2 p351.
 1 tpis91 PB  1.00F   2.00    0.00    0.00    0.00 1  245.1968064    -676000.000
    298.150    583.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15000.000
 1.363880730D+04 0.000000000D+00 7.104086710D+00 4.806777550D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -8.358963280D+04-2.908385050D+01
PbF2(I)          Cubic Crystal(I). TPIS 1991 v2 pt1 p421;pt2 p351.
 2 tpis91 PB  1.00F   2.00    0.00    0.00    0.00 2  245.1968064    -676000.000
    583.000    716.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15000.000
-7.862766420D+07 0.000000000D+00 1.154013530D+03-2.413080390D+00 1.453441510D-03
 0.000000000D+00 0.000000000D+00               -5.720487300D+05-6.285579570D+03
    716.000   1103.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15000.000
 3.516663040D+07 0.000000000D+00-1.580925390D+02 1.905776770D-01-5.650555480D-05
 0.000000000D+00 0.000000000D+00                4.370723820D+04 9.735936300D+02
PbF2(L)          Liquid. TPIS 1991 v2 pt1 p421;pt2 p351.
 1 tpis91 PB  1.00F   2.00    0.00    0.00    0.00 4  245.1968064    -676000.000
   1103.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15000.000
 0.000000000D+00 0.000000000D+00 1.310961200D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -8.458950020D+04-6.282775720D+01
PbI2(s)          Hexagonal Crystal. TPIS 1991 v2 pt1 p441;pt2 p366.
 2 tpis91 PB  1.00I   2.00    0.00    0.00    0.00 1  461.0089400    -176000.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19500.000
-6.615857400D+03 0.000000000D+00 8.879658690D+00 1.758307310D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.391562480D+04-3.012466440D+01
    298.150    683.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19500.000
 4.428402880D+04 0.000000000D+00 7.731062930D+00 3.690055100D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.348831170D+04-2.387008230D+01
PbI2(L)          Liquid. TPIS 1991 v2 pt1 p441;pt2 p366.
 1 tpis91 PB  1.00I   2.00    0.00    0.00    0.00 3  461.0089400    -176000.000
    683.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        19500.000
 0.000000000D+00 0.000000000D+00 1.310961200D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.355165610D+04-5.237973140D+01
PbO(II-r)        Tetragonal (II-red).TPIS 1991 v2 pt1 p409;pt2 p343.
 2 tpis91 PB  1.00O   1.00    0.00    0.00    0.00 1  223.1994000    -218600.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9225.000
 0.000000000D+00 0.000000000D+00 8.050624580D-01 2.884978163D-02-4.302158100D-05
 0.000000000D+00 0.000000000D+00               -2.743361905D+04-3.117085753D+00
    298.150    762.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9225.000
-6.651023332D+03 0.000000000D+00 4.939557472D+00 2.406636110D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.789339075D+04-2.073932502D+01
PbO(I-y)         Rhombic (I-yellow).TPIS 1991 v2 pt1 p409;pt2 p343.
 1 tpis91 PB  1.00O   1.00    0.00    0.00    0.00 3  223.1994000    -218600.000
    762.000   1160.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9225.000
-3.360390450D+04 0.000000000D+00 5.407414267D+00 1.595644241D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.802576574D+04-2.321766400D+01
PbO(L)           Liquid.TPIS 1991 v2 pt1 p409;pt2 p343.
 1 tpis91 PB  1.00O   1.00    0.00    0.00    0.00 4  223.1994000    -218600.000
   1160.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9225.000
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.664258145D+04-3.570913839D+01
PbO2(s)          Tetragonal Crystal.TPIS 1991 v2 pt1 p415;p52 p346.
 2 tpis91 PB  1.00O   2.00    0.00    0.00    0.00 1  239.1988000    -276000.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10962.000
 0.000000000D+00 0.000000000D+00 1.007530480D-01 4.035527600D-02-5.395750800D-05
 0.000000000D+00 0.000000000D+00               -3.454199070D+04-1.557803510D+00
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10962.000
-2.593057200D+05 0.000000000D+00 1.010402300D+01 5.003301460D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.709944890D+04-5.052640330D+01
PbS(cr)          Cubic Crystal. TPIS 1991 v2 pt1 p445;p52 p370.
 2 tpis91 PB  1.00S   1.00    0.00    0.00    0.00 1  239.2660000     -99474.800
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11510.000
-1.110196130D+04 0.000000000D+00 5.788552660D+00 9.715425300D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.377027529D+04-2.236417313D+01
    298.150   1386.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11510.000
-7.529006520D+04 0.000000000D+00 7.331760982D+00-2.262310106D-03 1.609234940D-06
 0.000000000D+00 0.000000000D+00               -1.431615352D+04-3.062514348D+01
PbS(L)           Liquid. TPIS 1991 v2 pt1 p445;p52 p370.
 1 tpis91 PB  1.00S   1.00    0.00    0.00    0.00 3  239.2660000     -99474.800
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   1386.500   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        11510.000
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.007241100D+04-3.316574241D+01
Pb2O3(s)         Monoclinic Crystal.TPIS 1991 v2 pt1 p417;pt2 p348.
 2 tpis91 PB  2.00O   3.00    0.00    0.00    0.00 1  462.3982000    -491700.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20880.000
 0.000000000D+00 0.000000000D+00 1.574967410D+00 6.633690300D-02-9.449445980D-05
 0.000000000D+00 0.000000000D+00                -6.172080000D+04-6.282642160D+00
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        20880.000
-3.314687210D+05 0.000000000D+00 1.505921580D+01 5.443495770D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.498118220D+04-7.101946640D+01
Pb3O4(cr)        Tetragonal Crystal.TPIS 1991 v2 pt1 p418;pt2 p349.
 1 tpis91 PB  3.00O   4.00    0.00    0.00    0.00 1  685.5976000    -720000.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        29830.000
 7.031601470D+06-8.770415980D+04 4.195886490D+02-9.058738460D-01 1.138287119D-03
-7.358926050D-07 1.922732625D-10                3.431611340D+05-2.394229365D+03
Rb(cr)           Rubidium Cubic Crystal. CODATA 1989. p260. JANAF 12/83.
 1 coda89 RB  1.00    0.00    0.00    0.00    0.00 1   85.4678000         0.000
    100.000    312.4707 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7489.000
-1.693678590D+05 5.116763890D+03-5.686760030D+01 3.403543090D-01-9.347995170D-04
 1.017512240D-06 0.000000000D+00                -2.164547070D+04 2.805350660D+02
Rb(L)            Rubidium Liquid. CODATA 1989. p260.
 2 coda89 RB  1.00    0.00    0.00    0.00    0.00 2   85.4678000         0.000
    312.470   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7489.000
 2.362394290D+04 2.869350480D+02 1.544988560D+00 5.168312170D-03-6.070292700D-06
 3.350636260D-09-5.185398910D-13                -1.935500990D+03 1.069559580D+00
   1000.000   2100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7489.000
-3.674486690D+05 1.779788690D+03-3.426046800D-01 5.323110980D-03-4.262806150D-06
 1.699804610D-09-4.418140260D-14                -1.111330670D+04 1.477905460D+01
RbOH(b)          Beta.  JPCRD v26 n4 1997 p1031.
 1 g 8/97 RB  1.00O   1.00H   1.00    0.00    0.00 1  102.4751400    -418800.000
    298.150    508.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13500.000
 0.000000000D+00 0.000000000D+00 6.589925323D+00 5.731305874D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.258929920D+04-2.794998878D+01
RbOH(c)          Gamma. JPCRD v26 n4 1997 p1031.
 1 g 8/97 RB  1.00O   1.00H   1.00    0.00    0.00 2  102.4751400    -418800.000
    508.000    658.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13500.000
 0.000000000D+00 0.000000000D+00 9.140646893D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.248404970D+04-3.962855491D+01
RbOH(L)          Liquid.JPCRD v26 n4 1997 p1031.
 1 g 8/97 RB  1.00O   1.00H   1.00    0.00    0.00 3  102.4751400    -418800.000
    658.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13500.000
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.231326390D+04-4.597096049D+01
S(cr1)           Sulfur Rhombic Crystal. TPIS 1989.
 1 tpis89 S   1.00    0.00    0.00    0.00    0.00 1   32.0660000         0.000
    200.000    368.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
-1.035710770D+04 0.000000000D+00 1.866766930D+00 4.256140290D-03-3.265252320D-06
 0.000000000D+00 0.000000000D+00                -7.516389560D+02-7.961066950D+00
S(cr2)           Sulfur Monoclinic Crystal. TPIS 1989.
 1 tpis89 S   1.00    0.00    0.00    0.00    0.00 2   32.0660000         0.000
    368.300    388.3607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
 0.000000000D+00 0.000000000D+00 2.080514130D+00 2.440879560D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.852714730D+02-8.607846750D+00
S(L)             Sulfur Liquid. TPIS 1989.
 5 tpis89 S   1.00    0.00    0.00    0.00    0.00 3   32.0660000         0.000
    388.360    428.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
-6.366550760D+07 0.000000000D+00 2.376860690D+03-7.888076030D+00 7.376076520D-03
 0.000000000D+00 0.000000000D+00                -6.356594920D+05-1.186929590D+04
    428.150    432.2507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
 0.000000000D+00 0.000000000D+00 6.928522310D+03-3.254655980D+01 3.824448180D-02
 0.000000000D+00 0.000000000D+00                -9.832222680D+05-3.154806750D+04
    432.250    453.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
 0.000000000D+00 0.000000000D+00 1.649945700D+02-6.843534980D-01 7.315907970D-04
 0.000000000D+00 0.000000000D+00                -2.638846930D+04-7.681730100D+02
    453.150    717.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
 1.972984580D+06 0.000000000D+00-2.441009750D+01 6.090352890D-02-3.744069100D-05
 0.000000000D+00 0.000000000D+00                 1.113013440D+04 1.363174180D+02
    717.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
 0.000000000D+00 0.000000000D+00 3.848693430D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.284589830D+02-1.736128240D+01
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SCL2(L)
 2 J 6/78 S   1.00CL  2.00    0.00    0.00    0.00 1  102.9714000     -49790.867
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.094524100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.251754300D+03-4.026979500D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.094524100D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.251754300D+03-4.026979500D+01
S2CL2(L)
 2 J 6/78 S   2.00CL  2.00    0.00    0.00    0.00 1  135.0374000     -58159.083
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.494893500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.145191500D+04-5.825022500D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.494893500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.145191500D+04-5.825022500D+01
Sc(a)           Alpha. TPIS 1982, v4, pt1, p137, pt2 p138.
 2 tpis82 SC  1.00    0.00    0.00    0.00    0.00 1   44.9559100         0.000
    100.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5207.000
-5.723537690D+03 0.000000000D+00 1.835072325D+00 9.478861990D-03-2.317188582D-05
 2.004221829D-08 0.000000000D+00               -8.225089040D+02-8.279121410D+00
    400.000   1609.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5207.000
-2.296409436D+04 0.000000000D+00 3.590296910D+00-1.480249906D-03 2.132230702D-06
-4.653598600D-10 0.000000000D+00               -1.099543829D+03-1.605255360D+01
Sc(b)           Beta. TPIS 1982, v4, pt1, p137, pt2 p138.
 1 tpis82 SC  1.00    0.00    0.00    0.00    0.00 2   44.9559100         0.000
   1609.000   1814.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5207.000
 0.000000000D+00 0.000000000D+00 5.316007798D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.113439951D+03-2.875686543D+01
Sc(l)           Liquid. TPIS 1982, v4, pt1, p137, pt2 p138.
 1 tpis82 SC  1.00    0.00    0.00    0.00    0.00 3   44.9559100         0.000
   1814.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5207.000
 0.000000000D+00 0.000000000D+00 5.291953464D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.373974847D+03-2.764152183D+01
Si(cr)          Silicon Cubic. TPIS 1991, v1, p237, v2, p220.
 2 tpis91 SI  1.00    0.00    0.00    0.00    0.00 1   28.0855000         0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3217.471
-2.323538210D+04 0.000000000D+00 2.102021680D+00 1.809220550D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -7.850635210D+02-1.038427320D+01
    298.150   1690.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3217.471
-5.232559730D+04 0.000000000D+00 2.850169420D+00 3.975166970D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.042947230D+03-1.438964190D+01
Si(L)           Silicon Liquid. TPIS 1991, v1, p237, v2, p220.
 1 tpis91 SI  1.00    0.00    0.00    0.00    0.00 2   28.0855000         0.000
   1690.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3217.471
 0.000000000D+00 0.000000000D+00 3.271389410D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                4.882667110D+03-1.326611070D+01
SiC(b)          Silicon Carbide Cubic Crystal(beta).TPIS,1991.
 1 tpis91 SI  1.00C   1.00    0.00    0.00    0.00 1   40.0962000    -73000.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3272.000
-2.285496380D+03 0.000000000D+00-5.349100620D-01 1.271547080D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.193174900D+03 1.241441350D+00
SiC(b)          Silicon Carbide Cubic Crystal(beta).TPIS,1991.
 1 tpis91 SI  1.00C   1.00    0.00    0.00    0.00 2   40.0962000    -73000.000
    298.150   3105.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3272.000
-1.269106660D+05 0.000000000D+00 3.757286960D+00 3.481744560D-03-1.620660750D-06
 2.611097950D-10 0.000000000D+00               -1.046667760D+04-2.109198540D+01
SiC(L)          Silicon Carbide Liquid.TPIS,1991.
 1 tpis91 SI  1.00C   1.00    0.00    0.00    0.00 3   40.0962000    -73000.000
   3103.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        3272.000
 0.000000000D+00 0.000000000D+00 7.577115190D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -7.787459000D+03-4.367596160D+01
SiO2(a-qz)      Hexagonal Crystal(alpha-quartz).TPIS 1991 v2 pt1 p250.
 1 tpis91 SI  1.00O   2.00    0.00    0.00    0.00 1   60.0843000   -910700.000
    200.000    848.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6916.000
-5.776895500D+05 7.214661110D+03-3.145730294D+01 7.412177150D-02-8.670077820D-06
-1.080461312D-07 8.316324910D-11               -1.462398375D+05 1.842424399D+02
SiO2(b-qz)      Hexagonal Crystal(beta-quartz). TPIS 1991 v2 pt1 p250.
 1 tpis91 SI  1.00O   2.00    0.00    0.00    0.00 2   60.0843000   -910700.000
    848.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6916.000
 2.317635074D+04 0.000000000D+00 7.026511484D+00 1.241925261D-03 0.000000000D+00
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 0.000000000D+00 0.000000000D+00              -1.117012474D+05-3.580751356D+01
SiO2(b-crt)      Cubic Crystal(beta-cristobalite).TPIS 1991 v2 pt1 p250.
 1 tpis91 SI  1.00O   2.00    0.00    0.00    0.00 3   60.0843000    -910700.000
   1200.000   1996.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6916.000
-5.356419079D+05 0.000000000D+00 9.331036946D+00-7.306503931D-04 3.339944266D-07
 0.000000000D+00 0.000000000D+00              -1.134326721D+05-4.998768383D+01
SiO2(L)          Liquid. TPIS 1991 v2 pt1 p250.
 1 tpis91 SI  1.00O   2.00    0.00    0.00    0.00 4   60.0843000    -910700.000
   1996.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6916.000
 0.000000000D+00 0.000000000D+00 1.004268442D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.140002976D+05-5.554279592D+01
SiS(cr)          Crystal. TPIS 1991 v2 pt1 p289; pt2 p257.
 1 tpis91 SI  1.00S   1.00    0.00    0.00    0.00 1   60.1515000    -168737.210
    298.150   1363.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9000.490
 0.000000000D+00 0.000000000D+00 4.873408054D+00 1.807202108D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.182763678D+04-2.072841584D+01
SiS(L)           Liquid. TPIS 1991 v2 pt1 p289; pt2 p257.
 1 tpis91 SI  1.00S   1.00    0.00    0.00    0.00 2   60.1515000    -168737.210
   1363.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        9000.490
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.076140696D+04-3.851581605D+01
SiS2(cr)         Tetragonal Crystal.TPIS 1991 v2 pt1 p293;pt2 p259.
 2 tpis91 SI  1.00S   2.00    0.00    0.00    0.00 1   92.2175000    -287000.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11180.490
-1.489679569D+04 0.000000000D+00 3.921710460D+00 1.226970632D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.628253940D+04-1.684224727D+01
    298.150   1363.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11180.490
 0.000000000D+00 0.000000000D+00 6.423349061D+00 3.317212921D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.658052990D+04-2.834259902D+01
SiS2(L)          Liquid.TPIS 1991 v2 pt1 p293;pt2 p259.
 1 tpis91 SI  1.00S   2.00    0.00    0.00    0.00 3   92.2175000    -287000.000
   1363.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       11180.490
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.909260770D+04-6.276638967D+01
Si2N2O(s)        Silicon Oxynitride. Fegley, CommAmCerSoc 1981 pC124-6.
 2 g 7/95 SI  2.00N   2.00O   1.00    0.00    0.00 1  100.1838800    -947700.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-7.783291740D+06 7.787696280D+04-3.226726620D+02 7.513787420D-01-9.139448890D-04
 5.774400830D-07-1.479973594D-10              -5.139864710D+05 1.873124085D+03
   1000.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-7.408337810D+06 2.557272171D+04-2.532253502D+01 3.206264920D-02-1.339020354D-05
 3.072315769D-09-2.890246453D-13              -2.761333204D+05 1.905530003D+02
Si3N4(cr)        Trisilicon Tetranitride Hexagonal Crystal(alpha).1991.
 2 tpis91 SI  3.00N   4.00    0.00    0.00    0.00 1  140.2834600    -787800.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12113.490
-1.136434510D+04 0.000000000D+00-4.993435710D-01 3.962318940D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.640037870D+04-1.086768950D+00
    298.150   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       12113.490
-2.910454130D+05 0.000000000D+00 1.189210190D+01 9.349799330D-03-2.551082390D-06
 2.857654870D-10 0.000000000D+00              -9.966541740D+04-6.412447980D+01
Sn(cr)           Tin CrI,tetragonal. TPIS 1991, pt1, p350, pt2, p300.
 1 tpis91 SN  1.00    0.00    0.00    0.00    0.00 1  118.7100000         0.000
    200.000    505.1187 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6323.000
-9.970244070D+05 1.864993890D+04-1.392956110D+02 5.652600010D-01-1.229117210D-03
 1.398206350D-06-6.465584700D-10              -8.479567560D+04 7.317726890D+02
Sn(L)            Tin Liquid. TPIS 1991, pt1, p350, pt2, p300.
 1 tpis91 SN  1.00    0.00    0.00    0.00    0.00 2  118.7100000         0.000
    505.118   4700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6323.000
 9.847844310D+04 0.000000000D+00 3.028921730D+00 2.531718650D-04-1.960428220D-08
 0.000000000D+00 0.000000000D+00               2.209651700D+02-9.089783770D+00
SnBr2(cr)        Rhombic Crystal. TPIS 1991 v2 pt1 p379;pt2 p322.
 2 tpis91 SN  1.00BR  2.00    0.00    0.00    0.00 1  278.5180000    -253600.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18670.000
-1.072142070D+04 0.000000000D+00 8.650388720D+00 3.246938990D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.326028440D+04-3.191324070D+01
    298.150    503.4007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18670.000
 1.596365870D+05 0.000000000D+00 4.310656910D+00 1.137469320D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.175626170D+04-8.652273970D+00
SnBr2(L)         Liquid. TPIS 1991 v2 pt1 p379;pt2 p322.
 2 tpis91 SN  1.00BR  2.00    0.00    0.00    0.00 3  278.5180000    -253600.000
    503.400    860.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18670.000
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 2.804494790D+05 0.000000000D+00 1.427732960D+01-2.218170400D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.305162210D+04-6.008238210D+01
   860.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18670.000
 0.000000000D+00 0.000000000D+00 1.274879700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.288346740D+04-5.185141220D+01
SnBr4(cr)        Monoclinic Crystal. TPIS 1991 v2 pt1 p382;pt2 p325.
 1 tpis91 SN  1.00BR  4.00    0.00    0.00    0.00 1  438.3260000    -388000.000
   200.000    302.2507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31260.000
-3.870038960D+06 0.000000000D+00 3.663330300D+02-1.775658617D+00 2.504656832D-03
 0.000000000D+00 0.000000000D+00              -1.120730416D+05-1.659626236D+03
SnBr4(L)         Liquid. TPIS 1991 v2 pt1 p382;pt2 p325.
 2 tpis91 SN  1.00BR  4.00    0.00    0.00    0.00 2  438.3260000    -388000.000
   302.250    470.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31260.000
 1.124780655D+05 0.000000000D+00 1.859869072D+01-4.792826035D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.036569340D+04-6.913668591D+01
   470.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31260.000
 0.000000000D+00 0.000000000D+00 1.888265213D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.079140710D+04-7.136367786D+01
SnCL2(cr)        Rhombic Crystal.TPIS 1991 v2 pt1 p372;pt2 p316.
 1 tpis91 SN  1.00CL  2.00    0.00    0.00    0.00 1  189.6154000    -333000.000
   200.000    520.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17330.000
-3.455659270D+05 5.121049170D+03-2.179939970D+01 8.738266180D-02-1.087380900D-04
 5.701191390D-08 0.000000000D+00              -6.692353190D+04 1.338412300D+02
SnCL2(L)         Liquid.TPIS 1991 v2 pt1 p372;pt2 p316.
 1 tpis91 SN  1.00CL  2.00    0.00    0.00    0.00 2  189.6154000    -333000.000
   520.200   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       17330.000
 0.000000000D+00 0.000000000D+00 1.322988370D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.294240400D+04-5.766924970D+01
SnCL4(L)         Tin Tetrachloride Liquid.TPIS,1991.
 2 tpis91 SN  1.00CL  4.00    0.00    0.00    0.00 1  260.5208000    -517000.000
   239.050    350.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38740.000
 0.000000000D+00 0.000000000D+00 2.059050980D+01-5.567014770D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.807207820D+04-8.378462340D+01
   350.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       38740.000
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -6.773111750D+04-7.431947540D+01
SnF2(cr)         Monoclinic Crystal.TPIS 1991 v2 pt1 p367;pt2 p311.
 1 tpis91 SN  1.00F   2.00    0.00    0.00    0.00 1  156.7068064    -677000.000
   298.150    488.2007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14200.000
 0.000000000D+00 0.000000000D+00 6.575252180D+00 7.150150760D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.370213250D+04-2.802481800D+01
SnF2(L)          Liquid.TPIS 1991 v2 pt1 p367;pt2 p311.
 1 tpis91 SN  1.00F   2.00    0.00    0.00    0.00 2  156.7068064    -677000.000
   488.200   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       14200.000
 0.000000000D+00 0.000000000D+00 1.202716700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.424882400D+04-5.569866810D+01
SnI2(cr)         Monoclinic Crystal. TPIS 1991 v2 pt1 p386;pt2 p328.
 1 tpis91 SN  1.00I   2.00    0.00    0.00    0.00 1  372.5189400    -153000.000
   200.000    595.7007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18950.000
 8.282713910D+05-1.299763600D+04 8.410445920D+01-1.990006290D-01 2.432175040D-04
-1.017853820D-07 0.000000000D+00               4.025330490D+04-4.484419650D+02
SnI2(L)          Liquid. TPIS 1991 v2 pt1 p386;pt2 p328.
 2 tpis91 SN  1.00I   2.00    0.00    0.00    0.00 2  372.5189400    -153000.000
   595.700    960.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18950.000
 3.807680790D+05 0.000000000D+00 1.313799610D+01-7.105650240D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.013981410D+04-5.193430840D+01
   960.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18950.000
 0.000000000D+00 0.000000000D+00 1.286906870D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.060570550D+04-5.097632390D+01
SnI4(cr)         Cubic Crystal. TPIS 1991 v2 pt1 p389;pt2 p331
 1 tpis91 SN  1.00I   4.00    0.00    0.00    0.00 1  626.3278800    -207500.000
   200.000    418.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31600.000
 1.365815910D+06-2.186441530D+04 1.411768650D+02-3.151970250D-01 2.991203130D-04
 0.000000000D+00 0.000000000D+00               7.347422110D+04-7.553382510D+02
SnI4(L)          Liquid. TPIS 1991 v2 pt1 p389;pt2 p331.
 2 tpis91 SN  1.00I   4.00    0.00    0.00    0.00 2  626.3278800    -207500.000
   418.000    580.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31600.000
 3.125499880D+05 0.000000000D+00 2.114568390D+01-5.918328320D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.828678880D+04-7.927900660D+01
   580.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       31600.000
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00
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 0.000000000D+00 0.000000000D+00              -2.836905730D+04-6.724586960D+01
SnO(cr)          Tetragonal Crystal.TPIS 1991 v2 pt1 p356; pt2 p306.
 2 tpis91 SN  1.00O   1.00    0.00    0.00    0.00 1  134.7094000    -280710.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8736.000
 0.000000000D+00 0.000000000D+00 7.279467580D-02 3.307685420D-02-4.710942000D-05
 0.000000000D+00 0.000000000D+00              -3.483713220D+04-1.306828650D+00
   298.150   1250.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8736.000
 0.000000000D+00 0.000000000D+00 5.260682830D+00 1.630883840D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.540242040D+04-2.358356590D+01
SnO(L)           Liquid.TPIS 1991 v2 pt1 p356; pt2 p306.
 1 tpis91 SN  1.00O   1.00    0.00    0.00    0.00 3  134.7094000    -280710.000
  1250.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8736.000
 0.000000000D+00 0.000000000D+00 7.577115190D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.369230760D+04-3.539798570D+01
SnO2(cr)         Tetragonal Crystal.TPIS 1991 v2 pt1 p361;pt2 p308.
 2 tpis91 SN  1.00O   2.00    0.00    0.00    0.00 1  150.7088000    -577630.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8384.000
 0.000000000D+00 0.000000000D+00-1.177647970D+00 3.970167880D-02-4.790758920D-05
 0.000000000D+00 0.000000000D+00              -7.046277710D+04 2.896556970D+00
   298.150   1903.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8384.000
-2.674601390D+05 0.000000000D+00 9.145457760D+00 8.856805750D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.313567410D+04-4.798106780D+01
SnO2(L)          Liquid.TPIS 1991 v2 pt1 p361;pt2 p308.
 1 tpis91 SN  1.00O   2.00    0.00    0.00    0.00 3  150.7088000    -577630.000
  1903.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8384.000
 0.000000000D+00 0.000000000D+00 1.106499360D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.222994130D+04-5.927455850D+01
SnS(rh)          Rhombic Crystal(I). TPIS 1991 v2 pt1 p392;pt2 p333.
 2 tpis91 SN  1.00S   1.00    0.00    0.00    0.00 1  150.7760000    -109662.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10530.000
-1.473490121D+04 0.000000000D+00 5.317316410D+00 2.586688381D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.493898062D+04-2.188910671D+01
   298.150    875.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10530.000
 3.056103126D+04 0.000000000D+00 4.511751143D+00 3.579405160D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.459100103D+04-1.734052255D+01
SnS(cu)          Cubic Crystal(I). TPIS 1991 v2 pt1 p392;pt2 p333.
 1 tpis91 SN  1.00S   1.00    0.00    0.00    0.00 3  150.7760000    -109662.000
   875.000   1154.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10530.000
 0.000000000D+00 0.000000000D+00 4.921516722D+00 1.882251630D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.425419920D+04-1.855922147D+01
SnS(L)           Liquid. TPIS 1991 v2 pt1 p392;pt2 p333.
 1 tpis91 SN  1.00S   1.00    0.00    0.00    0.00 4  150.7760000    -109662.000
  1154.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       10530.000
 0.000000000D+00 0.000000000D+00 9.008348057D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.391650549D+04-4.190990669D+01
SnS2(cr)         Hexagonal Crystal. TPIS 1991 v2 pt1 p396;pt2 p335.
 2 tpis91 SN  1.00S   2.00    0.00    0.00    0.00 1  182.8420000    -141837.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13310.000
-2.817980768D+04 0.000000000D+00 6.586339710D+00 7.259692260D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.943987500D+04-2.933754416D+01
   298.150   1143.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13310.000
 1.193094963D+04 0.000000000D+00 7.560277154D+00 2.479641013D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.938326475D+04-3.323586315D+01
Sr(a)            Alpha. JPCRD 1993 v22 n1 p1.
 2 srd 93 SR  1.00    0.00    0.00    0.00    0.00 1   87.6200000         0.000
   100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6558.289
-4.150245670D+03 1.559823384D+02-2.623173257D-01 2.945369354D-02-1.212940361D-04
 2.401045642D-07-1.708772572D-10              -1.455791066D+03 3.435106060D+00
   298.150    820.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6558.289
 1.294412876D+05-1.646179180D+03 1.111114164D+01-1.973737192D-02 2.910871519D-05
-2.163423606D-08 6.508160860D-12               7.160398040D+03-5.671602200D+01
Sr(b)            Beta. JPCRD 1993 v22 n1 p1.
 1 srd 93 SR  1.00    0.00    0.00    0.00    0.00 2   87.6200000         0.000
   820.000   1041.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6558.289
 0.000000000D+00 0.000000000D+00 3.190326309D+00 4.837326553D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.560991280D+02-1.157238431D+01
Sr(L)            Liquid. JPCRD 1993 v22 n1 p1.
 1 srd 93 SR  1.00    0.00    0.00    0.00    0.00 3   87.6200000         0.000
  1041.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6558.289
 0.000000000D+00 0.000000000D+00 4.450051777D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.431940390D+02-1.889703393D+01
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SrBr2(a)        CrII,tetragonal. TPIS 1996 pt1 p523 pt2 p403.
 1 tpis96 SR  1.00BR  2.00    0.00    0.00    0.00 1  247.4280000    -722000.000
    200.000    918.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18060.499
-1.563862878D+05 2.048387286D+03-2.389924996D+00 3.200996340D-02-4.324517230D-05
 3.247344210D-08-9.786717550D-12              -9.941922340D+04 2.897007516D+01
SrBr2(b)        CrI. TPIS 1996 pt1 p523 pt2 p403.
 1 tpis96 SR  1.00BR  2.00    0.00    0.00    0.00 2  247.4280000    -722000.000
    918.000    930.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18060.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -9.021650510D+04-5.212663905D+01
SrBr2(L)        Liquid. TPIS 1996 pt1 p523 pt2 p403.
 1 tpis96 SR  1.00BR  2.00    0.00    0.00    0.00 3  247.4280000    -722000.000
    930.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18060.499
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.900176120D+04-5.082046285D+01
SrCO3(a)        CrIII,rhombic. TPIS 1996 pt1 p532 pt2 p411.
 2 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 1  147.6289000   -1226000.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15120.499
-3.185109310D+07 5.983944250D+05-4.555778730D+03 1.807422903D+01-3.922550990D-02
 4.443338240D-05-2.057838162D-08              -2.840270234D+06 2.379927032D+04
    500.000   1198.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15120.499
-4.737741611D+05 0.000000000D+00 1.829247905D+01-1.342833192D-02 1.073412624D-05
 0.000000000D+00 0.000000000D+00              -1.539939771D+05-9.167197246D+01
SrCO3(b)        CrII,rhombic. TPIS 1996 pt1 p532 pt2 p411.
 1 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 3  147.6289000   -1226000.000
   1198.000   1689.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15120.499
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.541962605D+05-9.302015968D+01
SrCO3(c)        CrI,cubic. TPIS 1996 pt1 p532 pt2 p411.
 1 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 4  147.6289000   -1226000.000
   1689.000   1767.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15120.499
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.541962605D+05-9.302015968D+01
SrCO3(L)        Liquid. TPIS 1996 pt1 p532 pt2 p411.
 1 tpis96 SR  1.00C   1.00O   3.00    0.00    0.00 5  147.6289000   -1226000.000
   1767.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15120.499
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.534232745D+05-1.073837834D+02
SrCL2(a)        CrII,cubic.TPIS 1996 pt1 p518 pt2 p400.
 2 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 1  158.5254000    -833000.000
    200.000    700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16230.000
-8.219302560D+05 1.414627236D+04-9.066868860D+01 3.537351300D-01-6.601840230D-04
 6.294183590D-07-2.405335168D-10              -1.675299882D+05 4.920219760D+02
    700.000    990.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16230.000
 1.112527665D+09 0.000000000D+00-1.718772952D+04 4.254819093D+01-3.935556431D-02
 1.290928281D-05 0.000000000D+00               6.824931370D+06 9.213791630D+04
SrCL2(b)        CrI,cubic.TPIS 1996 pt1 p518 pt2 p400.
 1 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 3  158.5254000    -833000.000
    900.000   1147.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16230.000
 2.652616089D+08 0.000000000D+00-6.137593196D+02 3.705888862D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00               6.013938810D+05 4.028366895D+03
SrCL2(L)        Liquid.TPIS 1996 pt1 p518 pt2 p400.
 1 tpis96 SR  1.00CL  2.00    0.00    0.00    0.00 4  158.5254000    -833000.000
   1147.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        16230.000
-1.621863465D+06 0.000000000D+00 1.278463794D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.040518221D+05-6.010500872D+01
SrF2(a)         CrII,cubic.TPIS 1996 pt1 p513 pt2 p396.
 2 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 1  125.6168064   -1229000.000
    200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13075.000
-1.436181472D+04-3.902704550D+02 9.084528850D+00 4.747017010D-03-9.922331280D-06
 1.169135473D-08-4.825603120D-12              -1.484911532D+05-4.433988680D+01
    800.000   1484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13075.000
-1.706744719D+07 2.576630531D+04 3.257893350D+01-3.032276697D-02-2.832102640D-05
 2.982419101D-08-2.378577761D-12              -3.511043830D+05-1.514196992D+02
SrF2(b)         CrI,cubic.TPIS 1996 pt1 p513 pt2 p396.
 1 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 2  125.6168064   -1229000.000
   1484.000   1750.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13075.000
 5.274154560D+09-9.287005960D+04-1.188369557D+04 9.829240680D+00-2.277347958D-03
 0.000000000D+00 0.000000000D+00               1.339064905D+07 7.586298750D+04
SrF2(L)         Liquid.TPIS 1996 pt1 p515 pt2 p396.
 1 tpis96 SR  1.00F   2.00    0.00    0.00    0.00 3  125.6168064   -1229000.000
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   1750.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13075.000
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.478877648D+05-5.796718683D+01
SrH2(a)          CrII,rhombic. TPIS 1996 pt1 p501 pt2 p389.
 1 tpis96 SR  1.00H   2.00    0.00    0.00    0.00 1   89.6358800    -180000.000
   298.000   1128.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8000.499
 0.000000000D+00 0.000000000D+00 4.125438541D+00 3.912437414D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.305279501D+04-1.841745147D+01
SrH2(b)          CrI. TPIS 1996 pt1 p501 pt2 p389.
 1 tpis96 SR  1.00H   2.00    0.00    0.00    0.00 2   89.6358800    -180000.000
  1128.000   1323.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8000.499
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.467660041D+04-4.425795748D+01
SrH2(L)          Liquid. TPIS 1996 pt1 p501 pt2 p389.
 1 tpis96 SR  1.00H   2.00    0.00    0.00    0.00 3   89.6358800    -180000.000
  1323.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8000.499
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.254682969D+04-4.562495289D+01
SrI2(cr)         Rhombic. TPIS 1996 pt1 p527 pt2 p406.
 1 tpis96 SR  1.00I   2.00    0.00    0.00    0.00 1  341.4289400    -568000.000
   200.000    811.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18920.499
-8.531836590D+05 1.396294943D+04-8.134381170D+01 2.923620048D-01-4.941293260D-04
 4.280629170D-07-1.479234641D-10                -1.358835709D+05 4.559376890D+02
SrI2(L)          Liquid. TPIS 1996 pt1 p527 pt2 p406.
 1 tpis96 SR  1.00I   2.00    0.00    0.00    0.00 2  341.4289400    -568000.000
   811.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        18920.499
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.143040870D+04-5.646969655D+01
SrO(cr)          Cubic TPIS 1996 pt1 p494 pt2 p383.
 3 tpis96 SR  1.00O   1.00    0.00    0.00    0.00 1  103.6194000    -591000.000
   200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8680.499
-1.625438799D+06 2.932375088D+04-2.136643281D+02 8.526581540D-01-1.819594223D-03
 2.035599655D-06-9.340883290D-10                -2.053069998D+05 1.123784285D+03
   500.000   1800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8680.499
-3.410904551D+04 0.000000000D+00 5.049245235D+00 3.431471007D-03-3.042151612D-06
 9.069686608D-10 0.000000000D+00                -7.282782040D+04-2.317163697D+01
  1800.000   2805.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8680.499
-3.971117961D+07 0.000000000D+00 7.850733236D+01-5.336790743D-02 1.125297823D-05
 0.000000000D+00 0.000000000D+00                -1.604896850D+05-4.990588969D+02
SrO(L)           Liquid TPIS 1996 pt1 p494 pt2 p383.
 1 tpis96 SR  1.00O   1.00    0.00    0.00    0.00 4  103.6194000    -591000.000
  2805.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8680.499
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.188203330D+04-5.541556063D+01
Sr(OH)2(b)       CrII,tetragonal. TPIS 1996 pt1 p505 pt2 p392.
 1 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 1  121.6346800    -964300.000
   200.000    753.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15272.499
 5.749774650D+05-9.564782420D+03 6.310466570D+01-1.470270543D-01 2.468488663D-04
-2.041763520D-07 6.865596260D-11                -7.364279180D+04-3.424340180D+02
Sr(OH)2(a)       CrI. TPIS 1996 pt1 p505 pt2 p392.
 1 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 2  121.6346800    -964300.000
   753.000    808.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15272.499
 0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.216576455D+05-8.006737394D+01
Sr(OH)2(L)       Liquid. TPIS 1996 pt1 p505 pt2 p392.
 1 tpis96 SR  1.00O   2.00H   2.00    0.00    0.00 3  121.6346800    -964300.000
   808.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        15272.499
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.211265258D+05-9.516262078D+01
SrS(cr)          Cubic TPIS 1996 pt1 p528 pt2 p408.
 2 tpis96 SR  1.00S   1.00    0.00    0.00    0.00 1  119.6860000    -480000.000
   200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10040.499
 2.688173776D+06-5.010846740D+04 3.813026790D+02-1.462623236D+00 3.138875273D-03
-3.522660370D-06 1.619531388D-09                1.665724752D+05-1.992760719D+03
   500.000   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10040.499
-1.221960164D+04 0.000000000D+00 5.716873273D+00 9.316243531D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.951728090D+04-2.471633956D+01
SrS(L)           Liquid TPIS 1996 pt1 p528 pt2 p408.
 1 tpis96 SR  1.00S   1.00    0.00    0.00    0.00 3  119.6860000    -480000.000
  2500.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10040.499
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
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 0.000000000D+00 0.000000000D+00              -5.487727330D+04-3.767411768D+01
SrS04(a)        CrII,Rhombic. TPIS 1996 pt1 p531 pt2 p410.
 1 tpis96 SR  1.00S   1.00O   4.00    0.00    0.00 1  183.6836000   -1457000.000
    298.150   1430.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18400.499
-2.524863161D+05 0.000000000D+00 1.319271972D+01 6.424070691D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.803016041D+05-6.394942426D+01
SrS04(b)        CrI,hexagonal. TPIS 1996 pt1 p531 pt2 p410.
 1 tpis96 SR  1.00S   1.00O   4.00    0.00    0.00 2  183.6836000   -1457000.000
   1430.000   1880.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18400.499
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.827264862D+05-1.065597408D+02
SrS04(L)        Liquid. TPIS 1996 pt1 p531 pt2 p410.
 1 tpis96 SR  1.00S   1.00O   4.00    0.00    0.00 3  183.6836000   -1457000.000
   1880.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18400.499
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.783967061D+05-1.042566663D+02
Ta(cr)          Tantalum Crystal. JANAF Dec. 1972.
 3 j12/72 TA  1.00    0.00    0.00    0.00    0.00 1  180.9479000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5681.000
 1.519940430D+04-4.927141470D+02 6.855604420D+00-1.366625200D-02 2.561465720D-05
-2.235630670D-08 7.389829990D-12              1.236076770D+03-3.252074750D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5681.000
-1.001390000D+08 4.693014950D+05-8.986295820D+02 9.078786900D-01-5.040245690D-04
 1.463077630D-07-1.733477790D-11              -2.760103520D+06 5.935300910D+03
   2000.000   3258.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5681.000
 1.286248070D+05 5.624815940D+02-2.264086650D+00 6.791747120D-03-2.948975880D-06
 5.060666670D-10-8.391248130D-15              -1.570967590D+03 1.979982870D+01
Ta(L)           Tantalum Liquid. JANAF Dec. 1972.
 1 j12/72 TA  1.00    0.00    0.00    0.00    0.00 2  180.9479000         0.000
   3258.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5681.000
 0.000000000D+00 0.000000000D+00 5.032166660D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.436042050D+02-2.597362670D+01
TaC(s)
 2 J12/73 TA  1.00C   1.00    0.00    0.00    0.00 1  192.9586000    -144096.397
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.024971700D+00 1.762862000D-02-2.551585900D-05
 1.731330800D-08-4.305785800D-12              -1.822659700D+04-5.009312700D+00
   1000.000   4273.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.002705600D+00 1.284904100D-03-1.749593900D-07
 3.524558100D-11-2.642926000D-15              -1.902055300D+04-2.412969100D+01
TaC(L)
 1 J12/73 TA  1.00C   1.00    0.00    0.00    0.00 2  192.9586000         0.000
   4273.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.051671500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.010333800D+04-4.208554500D+01
Ta2O5(s)
 2 J12/72 TA  2.00O   5.00    0.00    0.00    0.00 1  441.8928000   -2046007.308
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.011994200D+01 2.553755900D-02-1.684735100D-05
 3.473407800D-11 3.126801100D-12              -2.500817400D+05-4.731087700D+01
   1000.000   2058.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.847368400D+01 3.490243300D-03 9.115658400D-07
-1.150828700D-09 2.470206000D-13              -2.524591100D+05-9.073349100D+01
Ta2O5(L)
 1 J12/72 TA  2.00O   5.00    0.00    0.00    0.00 2  441.8928000         0.000
   2058.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.918730900D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.533624500D+05-1.585777400D+02
Th(a)           Thorium Alpha Crystal. CODATA 1989. p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 1  232.0381000         0.000
    200.000   1650.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6350.000
-1.453247160D+04 1.505222440D+02 2.270694760D+00 2.058614360D-03-9.216614760D-07
 4.316796390D-10-7.950656890D-14              -1.667536360D+03-6.857176960D+00
Th(b)           Thorium Beta Crystal. CODATA 1989. p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 2  232.0381000         0.000
   1650.000   2023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6350.000
-4.483571080D+06 1.199959940D+04-1.099036560D+01 8.367713540D-03-1.870255340D-06
 2.025064490D-10 0.000000000D+00              -7.679626660D+04 8.908050670D+01
Th(L)           Thorium Liquid. CODATA 1989. p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 3  232.0381000         0.000
   2023.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        6350.000
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 0.000000000D+00 0.000000000D+00 5.532496800D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.191825100D+03-2.760071930D+01
Ti(a)          Titanium Alpha Crystal. CODATA 1989, p230.
 2 coda89 TI  1.00    0.00    0.00    0.00    0.00 1   47.8670000         0.000
    200.000    900.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4824.000
 3.598598660D+04-8.272301990D+02 7.689095440D+00-1.143967760D-02 1.392104390D-05
-4.691048580D-09-9.852157630D-13              2.936619540D+03-3.985136730D+01
    900.000   1156.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4824.000
-2.876235710D+06 0.000000000D+00 4.573153240D+01-7.692381330D-02 3.799919380D-05
 0.000000000D+00 0.000000000D+00              -2.038023870D+04-2.516270180D+02
Ti(b)          Titanium Beta Crystal. CODATA 1989, p230.
 1 coda89 TI  1.00    0.00    0.00    0.00    0.00 2   47.8670000         0.000
   1156.000   1944.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4824.000
-1.625891900D+06 6.281078300D+03-8.060150680D+00 9.348639300D-03-3.773463160D-06
 1.066055900D-09-1.138369620D-13              -3.752033730D+04 6.172942910D+01
Ti(L)          Titanium Liquid. CODATA 1989, p230.
 1 coda89 TI  1.00    0.00    0.00    0.00    0.00 3   47.8670000         0.000
   1944.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4824.000
 0.000000000D+00 0.000000000D+00 5.628714140D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.377354660D+03-3.079443480D+01
TiB(cr)         Crystal. JPCRD v15 sup1 1985 p256.
 2 j 6/65 TI  1.00B   1.00    0.00    0.00    0.00 1   58.6780000    -160247.000
    298.150   1100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 5.892962460D+05-7.628387170D+03 3.264504220D+01-4.438679670D-02 4.037756110D-05
-1.901806786D-08 3.662438970D-12              1.808566462D+04-1.924926707D+02
   1100.000   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 9.736238960D+05-2.744306202D+03 9.195602010D+00-1.636706129D-03 5.676930840D-07
-9.258425040D-11 6.105669480D-15              -3.925082340D+03-5.367424570D+01
TiB2(cr)        Crystal. JPCRD v15 sup1 1985 p276.
 2 j 6/65 TI  1.00B   2.00    0.00    0.00    0.00 1   69.4890000    -279491.000
    200.000   2300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5577.000
 2.701885716D+05-3.989107020D+03 1.904595810D+01-1.467951261D-02 1.249126541D-05
-4.481179720D-09 5.932523160D-13              -1.510818691D+04-1.130901290D+02
   2300.000   3193.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5577.000
 2.449855642D+10-5.420046130D+07 4.984385950D+04-2.437314870D+01 6.688502930D-03
-9.763538800D-07 5.923249200D-11              3.589528270D+08-3.651406280D+05
TiB2(L)         Liquid. JPCRD v15 sup1 1985 p276.
 1 j 6/65 TI  1.00B   2.00    0.00    0.00    0.00 2   69.4890000    -279491.000
   3193.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5577.000
 0.000000000D+00 0.000000000D+00 1.308363331D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -3.298172270D+04-7.649131141D+01
TiC(s)
 2 J 6/68 TI  1.00C   1.00    0.00    0.00    0.00 1   59.8777000    -184107.874
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.363394200D+00 2.825223700D-02-4.117521100D-05
 2.678885800D-08-6.346986800D-12              -2.267835200D+04 3.862648300D+00
   1000.000   3290.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.941393600D+00-3.727996700D-04 7.120995300D-07
-1.351709000D-10 9.980366000D-15              -2.417344500D+04-3.153022200D+01
TiC(L)
 1 J 6/68 TI  1.00C   1.00    0.00    0.00    0.00 2   59.8777000         0.000
   3290.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.548442100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.766020400D+04-4.062966100D+01
TiCL2(s)
 2 J12/68 TI  1.00CL  2.00    0.00    0.00    0.00 1  118.7724000    -515489.368
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.756751800D+00 1.363103300D-02-2.041622900D-05
 1.590988800D-08-4.545110400D-12              -6.416991800D+04-2.558545600D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.968414700D+00 2.544792500D-03-2.864811900D-07
 1.318780600D-10-2.227082600D-14              -6.450844200D+04-3.571308900D+01
TiCL3(s)
 2 J 6/68 TI  1.00CL  3.00    0.00    0.00    0.00 1  154.2251000    -721758.571
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.093793600D+01 2.662273600D-03-1.478592300D-07
-1.540676800D-09 9.221877400D-13              -9.018266800D+04-4.628728700D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.146265800D+01 1.401780600D-03-3.068972400D-08
 1.233900700D-13-1.056129800D-17              -9.031696000D+04-4.899307800D+01
TiCL4(L)
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 2 J12/67 TI  1.00CL  4.00    0.00    0.00    0.00 1  189.6778000    -804185.192
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.706604200D+01 1.577716800D-03-1.087037600D-06
 1.039030300D-09-3.602253000D-13              -1.018713400D+05-6.730822800D+01
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.714264300D+01 1.093708700D-03-1.069031100D-09
 2.661675700D-13-2.279448000D-17              -1.018802700D+05-6.764014200D+01
TiN(s)
 2 J 6/68 TI  1.00N   1.00    0.00    0.00    0.00 1   61.8737400    -337660.382
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.532011900D+00 4.117485600D-02-7.705577600D-05
 6.528986900D-08-2.060518700D-11              -4.112466600D+04 8.675079600D+00
   1000.000   3220.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.601005100D+00 3.564593900D-04 3.952180300D-07
-8.871800200D-11 7.784451300D-15              -4.244343000D+04-2.877329300D+01
TiN(L)
 1 J 6/68 TI  1.00N   1.00    0.00    0.00    0.00 2   61.8737400          0.000
   3220.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.548442100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.626170900D+04-3.958390600D+01
TiO(a)
 2 J12/73 TI  1.00O   1.00    0.00    0.00    0.00 1   63.8664000    -542676.363
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.980956400D-01 2.135438300D-02-3.584287300D-05
 3.040815700D-08-9.712163500D-12              -6.622433200D+04-5.956700400D+00
   1000.000   1265.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.651678500D+00 7.996320300D-03-4.955282800D-06
 1.412884200D-09 0.000000000D+00              -6.628836100D+04-1.291870300D+01
TiO(b)
 1 J12/73 TI  1.00O   1.00    0.00    0.00    0.00 2   63.8664000          0.000
   1265.000   2023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.797141900D+00 1.012886300D-02-7.458557100D-06
 3.083581500D-09-4.756174700D-13              -6.548277300D+04-7.934917500D+00
TiO(L)
 1 J12/73 TI  1.00O   1.00    0.00    0.00    0.00 3   63.8664000          0.000
   2023.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.051671500D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -6.327213800D+04-4.131210900D+01
TiO2(ru)
 2 J12/73 TI  1.00O   2.00    0.00    0.00    0.00 1   79.8658000    -944769.116
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.611751700D-01 3.796666000D-02-6.515475000D-05
 5.255213600D-08-1.620005100D-11              -1.147889700D+05-1.887403500D+00
   1000.000   2130.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.848915100D+00 4.246346100D-03-3.008898400D-06
 1.060251900D-09-1.437959700D-13              -1.159924600D+05-3.451410600D+01
TiO2(L)
 1 J12/73 TI  1.00O   2.00    0.00    0.00    0.00 2   79.8658000          0.000
   2130.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.207750700D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.149423000D+05-6.591075900D+01
Ti2O3(a)
 1 J 6/73 TI  2.00O   3.00    0.00    0.00    0.00 1  143.7322000   -1520834.429
    300.000    470.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.462354200D+01-3.716171700D-02 9.002647000D-05
 0.000000000D+00 0.000000000D+00               -1.864169300D+05-6.691489900D+01
Ti2O3(b)
 2 J 6/73 TI  2.00O   3.00    0.00    0.00    0.00 2  143.7322000          0.000
    470.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.697748500D+00 5.713743400D-02-8.332068100D-05
 5.729952800D-08-1.521168500D-11              -1.852503600D+05-1.406655900D+01
   1000.000   2115.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.487422200D+01 4.546569500D-03-2.364636300D-06
 5.996039200D-10-5.341426000D-14              -1.879734200D+05-7.786316500D+01
Ti2O3(L)
 1 J 6/73 TI  2.00O   3.00    0.00    0.00    0.00 3  143.7322000          0.000
   2115.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.887110500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.785869800D+05-9.656725700D+01
Ti3O5(a)
 1 J12/73 TI  3.00O   5.00    0.00    0.00    0.00 1  223.5980000   -2459221.144
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   300.000   450.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00-3.733743400D+00 1.061931900D-01-1.047238100D-04
 0.000000000D+00 0.000000000D+00              -2.984561700D+05 9.824101600D+00
Ti3O5(b)
 2 J12/73 TI  3.00O   5.00    0.00    0.00    0.00 2  223.5980000         0.000
   450.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.869281700D+01 8.505106200D-03-5.124620800D-06
 4.611987500D-09-1.523855700D-12              -3.001289500D+05-8.988958600D+01
  1000.000   2050.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 1.841515900D+01 8.001310200D-03-1.990705600D-06
 8.781239700D-10-1.424527500D-13              -2.999868400D+05-8.813547900D+01
Ti3O5(L)
 1 J12/73 TI  3.00O   5.00    0.00    0.00    0.00 3  223.5980000         0.000
  2050.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 3.220668600D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.936854100D+05-1.691270300D+02
Ti4O7(s)
 2 J12/73 TI  4.00O   7.00    0.00    0.00    0.00 1  303.4638000   -3404609.990
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00-8.633356000D-01 1.416046200D-01-2.324230500D-04
 1.819407300D-07-5.480141300D-11              -4.137948400D+05-4.563758000D+00
  1000.000   1950.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 2.411291500D+01 2.292771400D-02-1.711916300D-05
 6.484920600D-09-9.488381100D-13              -4.181071600D+05-1.210465000D+02
Ti4O7(L)
 1 J12/73 TI  4.00O   7.00    0.00    0.00    0.00 2  303.4638000         0.000
  1950.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 4.428419400D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.108967300D+05-2.351604300D+02
U(a)          Uranium Alpha Crystal. CODATA, 1989, p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 1  238.0289000         0.000
   200.000    942.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6364.000
-1.540899260D+04 2.318801680D+02 1.227944670D+00 7.136117000D-03-1.018038510D-05
 1.136884310D-08-3.669367260D-12              -1.986921730D+03-2.035975100D+00
U(b)          Uranium Beta Crystal. CODATA, 1989, p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 2  238.0289000         0.000
   942.000   1049.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6364.000
 0.000000000D+00 0.000000000D+00 5.099518790D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.672080150D+03-2.378030120D+01
U(c)          Uranium Gamma Crystal. CODATA, 1989, p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 3  238.0289000         0.000
  1049.000   1408.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6364.000
 0.000000000D+00 0.000000000D+00 4.606404950D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -5.859187280D+02-1.980809040D+01
U(L)          Uranium Liquid. CODATA, 1989, p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 4  238.0289000         0.000
  1408.000   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       6364.000
-9.464575870D+04 8.526093830D+02 4.209184450D+00 8.406886880D-04-1.309450110D-07
 1.984868960D-11-1.231477040D-15              -5.956058590D+03-1.667288210D+01
V(cr)         Vanadium Crystal. JANAF Jun.1973.
 3 j 6/73 V   1.00    0.00    0.00    0.00    0.00 1   50.9415000         0.000
   200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       4640.000
 2.845128550D+05-5.094937770D+03 3.715022350D+01-1.176032330D-01 2.255826430D-04
-2.260645830D-07 9.289610590D-11               2.254380420D+04-1.968243590D+02
   600.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       4640.000
 1.371659690D+06-7.844985770D+03 2.094461800D+01-2.054695350D-02 1.322539380D-05
-4.039247340D-09 5.082657380D-13               4.373372890D+04-1.292336490D+02
  1400.000   2190.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       4640.000
 3.010747300D+08-1.125907250D+06 1.747438610D+03-1.433039600D+00 6.592120870D-04
-1.607340270D-07 1.626691900D-11               6.867132370D+06-1.188589830D+04
V(L)          Vanadium Liquid. JANAF Jun.1973.
 1 j 6/73 V   1.00    0.00    0.00    0.00    0.00 2   50.9415000         0.000
  2190.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       4640.000
 0.000000000D+00 0.000000000D+00 5.557032220D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.899666730D+03-3.070530170D+01
VCL2(s)
 2 G 2/76 V   1.00CL  2.00    0.00    0.00    0.00 1  121.8469000   -451882.134
   300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
 0.000000000D+00 0.000000000D+00 6.739559900D+00 1.048722300D-02-1.722678000D-05
 1.476883100D-08-4.755070600D-12              -5.669888600D+04-2.920570400D+01
  1000.000   1300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
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 0.000000000D+00 0.000000000D+00 6.271121600D+00 7.489004600D-03-5.253100000D-06
 1.506736900D-09 0.000000000D+00              -5.635805600D+04-2.572653800D+01
VCL3(s)
 1 G 2/76 V   1.00CL  3.00    0.00    0.00    0.00 1  157.2996000    -580750.741
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.977041300D+00 2.354201100D-02-4.074527200D-05
 3.492848300D-08-1.124490000D-11              -7.267816900D+04-2.949371200D+01
VCL4(L)
 2 G 2/76 V   1.00CL  4.00    0.00    0.00    0.00 1  192.7523000    -569456.890
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.746206300D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.369584500D+04-6.879479200D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.746206300D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.369584500D+04-6.879479200D+01
VN(s)
 2 J12/73 V   1.00N   1.00    0.00    0.00    0.00 1   64.9482400    -217151.453
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.127135700D-01 2.010104300D-02-3.117800400D-05
 2.310368900D-08-6.384514400D-12              -2.702009400D+04-4.945743600D+00
   1000.000   3500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.836874000D+00 1.890014700D-03-3.161046300D-07
 4.605066000D-11-1.910203700D-15              -2.773815200D+04-2.387335300D+01
VO(s)
 2 J12/73 V   1.00O   1.00    0.00    0.00    0.00 1   66.9409000    -431782.448
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.538040100D+00 1.644707800D-02-2.855981000D-05
 2.483639200D-08-7.988694800D-12              -5.321191900D+04-1.359975800D+01
   1000.000   2063.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.339871500D+00 1.759170300D-03 3.847761700D-07
-2.618247100D-10 5.100939500D-14              -5.365137900D+04-2.638236400D+01
VO(L)
 1 J12/73 V   1.00O   1.00    0.00    0.00    0.00 2   66.9409000         0.000
   2063.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.548442100D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.760047400D+04-3.615421300D+01
V2O3(s)
 2 J12/73 V   2.00O   3.00    0.00    0.00    0.00 1  149.8812000   -1218793.074
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.287703300D+00 5.763276300D-02-9.673855600D-05
 7.406691600D-08-2.065838900D-11              -1.491118900D+05-1.472344600D+01
   1000.000   2340.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.396421100D+01 1.687129800D-03 1.137120600D-06
-2.080600700D-10 1.002832500D-14              -1.510057500D+05-6.878289400D+01
V2O3(L)
 1 J12/73 V   2.00O   3.00    0.00    0.00    0.00 2  149.8812000         0.000
   2340.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.887110500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.403406300D+05-9.458092000D+01
V2O4(I)
 1 J 6/73 V   2.00O   4.00    0.00    0.00    0.00 1  165.8806000   -1427198.055
    300.000    340.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 6.891454200D+00 9.914202200D-03 5.783710100D-05
 4.305391900D-08-2.848269400D-10              -1.746086400D+05-3.215735800D+01
V2O4(II)
 2 J 6/73 V   2.00O   4.00    0.00    0.00    0.00 2  165.8806000         0.000
    340.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 4.900362400D+00 5.002695200D-02-7.131633200D-05
 4.651556700D-08-1.078326800D-11              -1.737367600D+05-2.450337500D+01
   1000.000   1818.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.661025600D+01 2.332941900D-03 9.890478600D-07
-7.503249600D-10 1.613546100D-13              -1.760738900D+05-8.083199700D+01
V2O4(L)
 1 J 6/73 V   2.00O   4.00    0.00    0.00    0.00 3  165.8806000         0.000
   1818.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.566470300D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.746300900D+05-1.365594000D+02
V2O5(s)
 1 J 6/73 V   2.00O   5.00    0.00    0.00    0.00 1  181.8800000   -1550616.106
    300.000    943.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-1.164036000D+00 9.353588400D-02-1.567509700D-04
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 1.222352400D-07-3.573884500D-11              -1.891453100D+05 4.072275300D-01
V2O5(L)
 2 J 6/73 V   2.00O   5.00    0.00    0.00    0.00 2  181.8800000         0.000
    943.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.294726400D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.875144700D+05-1.108927700D+02
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.294726400D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.875144700D+05-1.108927700D+02
W(cr)           Tungsten Crystal. JANAF Jun.1966.
 4 j 6/66 W   1.00    0.00    0.00    0.00    0.00 1  183.8400000         0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4973.000
-6.824554640D+03-2.254247220D+02 4.976603540D+00-6.926433280D-03 1.202272520D-05
-9.344129990D-09 2.818886060D-12              -3.511569840D+00-2.361334390D+01
   1000.000   2600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4973.000
 5.528862940D+05-2.041000160D+03 5.870085660D+00-1.920103460D-03 1.067380740D-06
-2.354475540D-10 2.160077650D-14              1.163517100D+04-3.318658350D+01
   2600.000   3200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4973.000
 1.923119210D+10-3.036369850D+07 1.781339880D+04-4.238576610D+00 5.064416930D-05
 1.399725310D-07-1.658462900D-11              2.126725340D+08-1.400976890D+05
   3200.000   3680.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4973.000
 3.789946540D+10-6.895552180D+07 4.817632890D+04-1.634431240D+01 2.711729880D-03
-1.766853790D-07 0.000000000D+00              4.729192110D+08-3.681648660D+05
W(L)            Tungsten Liquid. JANAF Jun.1966.
 1 j 6/66 W   1.00    0.00    0.00    0.00    0.00 2  183.8400000         0.000
   3680.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        4973.000
 0.000000000D+00 0.000000000D+00 4.277341660D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              2.755414890D+03-2.086448920D+01
WC(cr)          Barin 1989. Hf:JPCRD v11 1982 sup2.
 1 bar 89 W   1.00C   1.00    0.00    0.00    0.00 1  195.8507000    -40540.000
    298.150   2500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-1.119754391D+05-5.553268210D-01 5.217965240D+00 1.037888263D-03-1.229060652D-07
 2.880427321D-13-7.236307119D-17             -6.848998700D+03-2.677066218D+01
WCL6(I)         Alpha1. JANAF 12/66. JPCRD v14 sup1 1985.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 1  396.5562000    -593710.000
    298.150    450.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 1.661826519D+02 0.000000000D+00 1.508873100D+01 2.015651227D-02-2.754798370D-08
 0.000000000D+00 0.000000000D+00              -7.680028810D+04-6.329365920D+01
WCL6(II)        Alpha2. JANAF 12/66. JPCRD v14 sup1 1985.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 2  396.5562000    -593710.000
    450.000    503.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-9.897046360D+03 0.000000000D+00 1.522857952D+01 1.994376611D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.636166220D+04-6.296167010D+01
WCL6(III)       Beta. JANAF 12/66. JPCRD v14 sup1 1985.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 3  396.5562000    -593710.000
    503.000    555.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.264474996D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.565217840D+04-9.527165358D+01
WCL6(L)         Liquid. JANAF 12/66. JPCRD v14 sup1 1985.
 1 j12/66 W   1.00CL  6.00    0.00    0.00    0.00 4  396.5562000    -593710.000
    555.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.415439996D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.568493560D+04-1.033604557D+02
WOCL4(cr)       JANAF 3/67. JPCRD v14 sup1 1985.
 1 j 3/67 W   1.00O   1.00CL  4.00    0.00    0.00 1  341.6502000    -671114.000
    298.150    484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 1.295153216D+03 0.000000000D+00 1.378522135D+01 1.276179773D-02-1.713279395D-07
 0.000000000D+00 0.000000000D+00              -8.538742740D+04-6.154983780D+01
WOCL4(L)        Liquid. JANAF 3/67. JPCRD v14 sup1 1985.
 1 j 3/67 W   1.00O   1.00CL  4.00    0.00    0.00 2  341.6502000    -671114.000
    484.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -8.236656270D+04-9.422321377D+01
WO2(cr)         TPIS 1982 pt1 p39,46 pt2 p49.
 1 tpis82 W   1.00O   2.00    0.00    0.00    0.00 1  215.8388000    -588100.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8711.000
-1.733842408D+04 0.000000000D+00 2.558979845D+00 1.457260175D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.220058630D+04-1.293182268D+01
WO2(cr)         TPIS 1982 pt1 p39,46 pt2 p49.
 1 tpis82 W   1.00O   2.00    0.00    0.00    0.00 2  215.8388000    -588100.000
    298.150   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8711.000
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-1.555714047D+05 0.000000000D+00 7.983272616D+00 1.595163155D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -7.370467050D+04-4.074555290D+01
WO2CL2(cr)       JANAF 3/67. JPCRD v14 sup1 1985.
 1 j 3/67 W   1.00O   2.00CL  2.00    0.00    0.00 1  286.7442000    -780316.000
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-3.819410020D+05 2.367029691D+03 9.834455770D+00-2.508443012D-02 1.017169638D-04
-1.040117941D-07 3.468311980D-11              -1.111440350D+05-2.227929881D+01
WO3(crIII)       TPIS 1982 pt1 p39,49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 1  231.8382000    -841300.000
    100.000    325.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13280.000
-2.841140443D+05 7.257714840D+03-6.708405120D+01 3.092936300D-01-4.127635650D-04
 0.000000000D+00 0.000000000D+00              -1.335884160D+05 3.409113710D+02
WO3(crIII,II)    TPIS 1982 pt1 p39,49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 2  231.8382000    -841300.000
    325.000   1013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13280.000
-5.186114395D+04 0.000000000D+00 8.548308920D+00 4.317151582D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.040935177D+05-4.044670662D+01
WO3(crI)         TPIS 1982 pt1 p39,49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 3  231.8382000    -841300.000
   1013.000   1747.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13280.000
 0.000000000D+00 0.000000000D+00 9.737555190D+00 1.958624140D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.039166330D+05-4.614390358D+01
WO3(L)           Liquid TPIS 1982 pt1 p39,49 pt2 p51.
 1 tpis82 W   1.00O   3.00    0.00    0.00    0.00 4  231.8382000    -841300.000
   1747.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       13280.000
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.022412072D+05-8.082927535D+01
Zn(cr)           Zinc Crystal. CODATA 1989, p221.
 1 coda89 ZN  1.00    0.00    0.00    0.00    0.00 1   65.3900000         0.000
    200.000    692.7307 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5657.000
 3.702054180D+05-5.915431780D+03 3.959471110D+01-1.143725810D-01 1.934344970D-04
-1.675366970D-07 6.078119330D-11               2.681717030D+04-2.114832510D+02
Zn(L)            Zinc Liquid. CODATA 1989, p221.
 1 coda89 ZN  1.00    0.00    0.00    0.00    0.00 2   65.3900000         0.000
    692.730   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5657.000
 0.000000000D+00 0.000000000D+00 3.776530430D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -4.317345810D+02-1.567077930D+01
ZnSO4(a)
 1 J 3/79 ZN  1.00S   1.00O   4.00    0.00    0.00 1  161.4536000    -980151.048
    300.000    540.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.165736400D+00 2.397739400D-02-3.070074400D-06
-4.845016400D-09 0.000000000D+00              -1.204535900D+05-2.310536900D+01
ZnSO4(a)
 2 J 3/79 ZN  1.00S   1.00O   4.00    0.00    0.00 2  161.4536000         0.000
    540.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.555349500D+01 2.773731900D-03-3.803472100D-06
 4.084554300D-09-1.528956200D-12              -1.225049000D+05-7.622168400D+01
   1000.000   1013.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.589525900D+01 1.184094200D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.226043300D+05-7.791532200D+01
ZnSO4(b)
 1 J 3/79 ZN  1.00S   1.00O   4.00    0.00    0.00 3  161.4536000         0.000
   1013.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.746182500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.211380600D+05-8.514325300D+01
Zr(a)            Zirconium Alpha Crystal.  JANAF Jun.1979.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 1   91.2240000         0.000
    200.000   1135.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5497.000
-1.153699590D+04 2.626208630D+01 2.932054420D+00 5.743366140D-04-7.651721000D-07
 1.597203570D-09-6.097131650D-13              -1.084153510D+03-1.215776800D+01
Zr(b)            Zirconium Beta Crystal.  JANAF Jun.1979.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 2   91.2240000         0.000
   1135.000   2125.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5497.000
-1.062988700D+06 4.263263380D+03-3.158058440D+00 5.005309000D-03-2.356975400D-06
 7.691317180D-10-8.139248310D-14              -2.635355160D+04 3.061359550D+01
Zr(L)            Zirconium Liquid.  JANAF Jun.1979.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 3   91.2240000         0.000
   2125.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        5497.000
 0.000000000D+00 0.000000000D+00 5.032166660D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -1.100795870D+03-2.548066000D+01
ZrN(s)
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 2 J 6/61 ZR  1.00N   1.00    0.00    0.00    0.00 1  105.2307400    -365249.014
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 2.855629000D+00 8.616697000D-03-5.348663800D-06
-2.880421900D-09 3.108784900D-12               -4.511202000D+04-1.390106900D+01
   1000.000   3225.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 5.540782000D+00 6.183935300D-04 2.954211000D-07
-1.178431100D-10 1.524143000D-14               -4.575132400D+04-2.742065400D+01
ZrN(L)
 1 J 6/61 ZR  1.00N   1.00    0.00    0.00    0.00 2  105.2307400         0.000
   3225.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 7.045116400D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.810552700D+04-3.443626400D+01
ZrO2(a)
 2 J12/65 ZR  1.00O   2.00    0.00    0.00    0.00 1  123.2228000   -1097471.394
    300.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-7.953710600D-01 4.393345800D-02-8.121444400D-05
 6.956764800D-08-2.238094700D-11               -1.331196700D+05 5.322100900D-01
   1000.000   1478.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00-2.214439500D+01 9.963976300D-02-1.200668800D-04
 6.468673600D-08-1.300488100D-11               -1.273279700D+05 1.110089100D+02
ZrO2(b)
 1 J12/65 ZR  1.00O   2.00    0.00    0.00    0.00 2  123.2228000         0.000
   1478.000   2950.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 8.957362900D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.341435400D+05-4.527401700D+01
ZrO2(L)
 1 J12/65 ZR  1.00O   2.00    0.00    0.00    0.00 3  123.2228000         0.000
   2950.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 0.000000000D+00 0.000000000D+00 1.056767500D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.284274500D+05-5.459226400D+01
Air             Mole%:N2 78.084,O2 20.9476,Ar .9365,CO2 .0319.NASA TP1906 1982
 2 g 9/95 N   1.56O   0.42AR  0.01C   0.00    0.00 0   28.9651784      -125.530
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8649.264
 1.009950160D+04-1.968275610D+02 5.009155110D+00-5.761013730D-03 1.066859930D-05
-7.940297970D-09 2.185231910D-12               -1.767967310D+02-3.921500990D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        8649.264
 2.415214430D+05-1.257874600D+03 5.144558670D+00-2.138541790D-04 7.065227840D-08
-1.071483490D-11 6.577800150D-16               6.462263190D+03-8.147408670D+00
B2H6(L)          Diborane. JANAF Prop.Ser.E,1/67. TPIS v.III,1981.
 0 g 4/95 B   2.00H   6.00    0.00    0.00    0.00 1   27.6696400      16445.000
    180.590      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
B5H9(L)          Pentaborane. JANAF June 1963 p300.
 0 j 6/63 B   5.00H   9.00    0.00    0.00    0.00 1   63.1264600      42840.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
(CH2)x(s)        Ethylene polymer. Est.from paraffin HC series,TRC p-2500,4/88.
 0 g 4/95 C   1.00H   2.00    0.00    0.00    0.00 1   14.0268800     -25600.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
CH3NO2(L)        Nitromethane. TRC p-9520,12/91.
 0 x12/91 C   1.00H   3.00N   1.00O   2.00    0.00 1   61.0403600    -113100.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
CH4(L)           Methane. TRC m-1350,10/93. JANAF Prop.Ser.E,1/67.
 0 g 4/95 C   1.00H   4.00    0.00    0.00    0.00 1   16.0427600     -89233.000
    111.643      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
CH3OH(L)         Methanol. TRC p-5000,12/87; tc,uc,vc-5031-3,12/84.
 1 x12/84 C   1.00H   4.00O   1.00    0.00    0.00 1   32.0418600    -238910.000
    175.610    390.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       18995.000
-1.302005180D+06 3.166985230D+04-3.031243150D+02 1.602231630D+00-4.594508740D-03
 6.990180370D-06-4.207390190D-09               -1.656168650D+05 1.514347140D+03
CH6N2(L)         Monomethyl Hydrazine. TRC p-9220,12/93.
 0 x12/93 C   1.00H   6.00N   2.00    0.00    0.00 1   46.0721200      54200.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C2H2(L),acetyle   Acetylene. JANAF Prop.Ser.E,1/67. TRC a-3000,10/86.
 0 g 3/95 C   2.00H   2.00    0.00    0.00    0.00 1   26.0378800     207599.000
    192.350      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
CH3CN(L)         Ethanenitrile (Acetonitrile). JPCRD v11,Sup.2,1982.
 0 g 3/95 C   2.00H   3.00N   1.00    0.00    0.00 1   41.0525600      31380.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C2H4(L)          Ethylene. TRC m-2600,10/93.
 0 g 4/95 C   2.00H   4.00    0.00    0.00    0.00 1   28.0537600      33945.000
    169.420      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C2H4O(L),ethyle   Ethylene oxide (Oxirane). TRC m-6150,6/94.
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 0 g 4/95 C   2.00H   4.00O   1.00    0.00    0.00 1   44.0531600     -78841.000
    283.650     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C2H6(L)          Ethane. TRC m-1350, 10/93.
 0 g 4/95 C   2.00H   6.00    0.00    0.00    0.00 1   30.0696400    -103819.000
    184.559     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C2H5OH(L)        TRC p-5000,12/31/87; tc,uc,vc-5031-3,12/31/84.
 1 x12/84 C   2.00H   6.00O   1.00    0.00    0.00 1   46.0684400    -277510.000
    159.000   390.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       24082.000
 4.501115940D+05-1.020828990D+04 1.014266780D+02-3.874672610D-01 7.121392610D-04
-1.857071450D-07-2.037622570D-10                7.448557900D+03-5.044255520D+02
C2H8N2(L),UDMH    Unsymmetrical Dimethyl Hydrazine. TRC p9220,12/93.
 0 g 4/95 C   2.00H   8.00N   2.00    0.00    0.00 1   60.0990000     48900.000
    298.150     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C2N2(L)          Cyanogen. Hdbk C&P Ed.73,1992-3.
 0 g 3/95 C   2.00N   2.00    0.00    0.00    0.00 1   52.0354800    283209.000
    252.050     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C3H6(L),propyle   Propylene. TRC m2600,10/93.
 0 g 4/95 C   3.00H   6.00    0.00    0.00    0.00 1   42.0806400      -2704.000
    225.460     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C3H7NO3(L)       Propyl Nitrate. Pedley,Naylor,Kirby,1986 p178.
 0 g 4/95 C   3.00H   7.00N   1.00O   3.00    0.00 1  105.0935200    -214500.000
    298.150     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C3H8(L)          Propane. TRC m1350,10/93.
 0 g 4/95 C   3.00H   8.00    0.00    0.00    0.00 1   44.0965200    -128228.000
    231.076     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C4H8(L),1-buten   1-Butene. TRC m-2600,10/93. p-2600,4/88.
 0 g 3/95 C   4.00H   8.00    0.00    0.00    0.00 1   56.1075200     -25173.000
    266.920     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C4H10(L),n-buta   n-Butane. TRC m-1350,10/93.
 0 g 3/95 C   4.00H  10.00    0.00    0.00    0.00 1   58.1234000    -150664.000
    272.638     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C4H10(L),isobut   Isobutane(2-methyl propane). TRC m-1350,10/93.
 0 g 3/95 C   4.00H  10.00    0.00    0.00    0.00 1   58.1234000    -159664.000
    261.361     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C5H12(L),n-pent   n-Pentane. TRC p-1350,4/85.
 0 g 4/85 C   5.00H  12.00    0.00    0.00    0.00 1   72.1502800    -173490.000
    298.150     0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
C6H6(L)          Benzene. TRC tc,uc,vc-3201,10/31/86; p-3200,4/30/83.
 1 x10/86 C   6.00H   6.00    0.00    0.00    0.00 1   78.1118400      49080.000
    278.680   500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       30110.000
-2.560137100D+06 4.136745880D+04-2.122973570D+02 3.723579020D-01 7.561068870D-04
-3.077215090D-06 2.787506250D-09               -1.935467780D+05 1.231845750D+03
C6H5NH2(L)       Aniline. TRC p9370 6/30/90. TRC tc,uc,vc-9370 12/31/88
 1 x12/88 C   6.00H   7.00N   1.00    0.00    0.00 1   93.1265200      31500.000
    267.130   460.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       34020.000
 6.267734410D+07-8.947510400D+05 5.067615710D+03-1.402163200D+01 1.899635910D-02
-9.316664840D-06-1.238222490D-09                4.275410610D+06-2.807774080D+04
C6H14(L),n-hexa   n-hexane. TRC p,tc,uc,vc-1440-1,4/85.
 1 x 4/85 C   6.00H  14.00    0.00    0.00    0.00 1   86.1753600    -198660.000
    177.860   300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       46920.000
 7.730917160D+06-2.251892470D+05 2.719902840D+03-1.699867070D+01 5.912397590D-02
-1.075409440D-04 8.030437090D-08                8.819466380D+05-1.294138410D+04
C7H8(L)          TRC tc,uc,vc-3200-1,10/31/86; p-3200,4/30/83.
 1 x10/86 C   7.00H   8.00    0.00    0.00    0.00 1   92.1384200      12180.000
    178.150   500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       33470.000
-3.713560030D+06 7.772550720D+04-6.312287990D+02 2.724399860D+00-6.103553860D-03
 7.022445240D-06-3.113727500D-09               -3.452125050D+05 3.265990010D+03
C7H16(L),n-hept   TRC m-1460,4/93; tc,uc,vc-1460,10/31/75.
 1 x10/75 C   7.00H  16.00    0.00    0.00    0.00 1  100.2019400    -224350.000
    182.580   380.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       52640.000
 1.760036000D+06-3.749601730D+04 3.963259800D+02-2.117924980D+00 6.828519710D-03
-1.131901770D-05 7.737098830D-09                1.269160320D+05-1.921784190D+03
C8H18(L),n-octa   TRC tables tc,uc,vc-1491-2. Hf298: p-1010,Oct.31,1984.
 1 x10/76 C   8.00H  18.00    0.00    0.00    0.00 1  114.2285200    -250260.000
    216.370   310.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       61490.000
-2.322825010D+07 4.846535450D+05-4.084818230D+03 1.820819280D+01-4.465662900D-02
 5.814101340D-05-3.149603340D-08               -2.166270480D+06 2.091659730D+04
C8H18(L),isooct   TRC tables tc,uc,vc-1491-2. Hf298: p-1490,Oct.31,1982.
 1 x10/76 C   8.00H  18.00    0.00    0.00    0.00 1  114.2285200    -259160.000
    165.790   380.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0       50190.000
 4.781047660D+06-1.126911380D+05 1.096521770D+03-5.344117040D+00 1.460037240D-02
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-2.028719990D-05 1.133400430D-08              4.432848740D+05-5.457905150D+03
CLF3(L)          JANAF Prop.SerD,3/66. TRC k-140,12/73.
 0 g 3/95 CL  1.00F   3.00    0.00    0.00    0.00 1   92.4479100    -193386.000
    284.890      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
CLO3F            Perchloryl Fluoride. JPCRD v22 sup2,1982. JANAF 3/61.
 2 g 5/95 CL  1.00O   3.00F   1.00    0.00    0.00 0  102.4493032     -23800.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13298.823
 4.460877700D+04-5.892084080D+02 3.558713370D+00 2.809620190D-02-3.610924770D-05
 2.273360160D-08-5.716802720D-12              -1.388798110D+03 4.591513620D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13298.823
-3.910413440D+05-1.193259020D+03 1.388663300D+01-3.541683980D-04 7.826598350D-08
-8.979916880D-12 4.164698430D-16              -1.274851990D+03-5.106493440D+01
CLO3F(L)         Perchloryl Fluoride. Hdbk C&P,ED.73,1992-3.
 0 g 4/95 CL  1.00O   3.00F   1.00    0.00    0.00 1  102.4493000     -47436.000
    226.400      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
CL2(L)           Chlorine. HdbkC&P Ed.73,1992-3. JANAF Prop.Ser.E,1/67
 0 g 4/95 CL  2.00    0.00    0.00    0.00    0.00 1   70.9054000     -22550.000
    239.120      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
F2(L)            Fluorine. Hdbk C&P Ed.73 1992-3. JANAF Prop.Ser.D,3/66.
 0 g 4/95 F   2.00    0.00    0.00    0.00    0.00 1   37.9968100     -13091.000
     85.020      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
F2O(L)           Oxygen Difluoride.Hdbk C&P Ed.73,1992-3.JANAF Prop.Ser.E,1/67.
 0 g 4/95 F   2.00O   1.00    0.00    0.00    0.00 1   53.9962100       6672.000
    128.400      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
HNO3(L)          Nitric Acid. Hdbk C&P Ed.73,1992-3,p6-102.
 0 g 4/95 H   1.00N   1.00O   3.00    0.00    0.00 1   63.0128800    -173013.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
H2(L)            Hydrogen. JANAF Prop.Ser.D,3/66.
 0 jp3/66 H   2.00    0.00    0.00    0.00    0.00 1    2.0158800      -9012.000
     20.270      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
H2O2(L)          Hydrogen Peroxide Liquid.TPIS,1989.
 1 tpis89 H   2.00O   2.00    0.00    0.00    0.00 1   34.0146800    -187780.000
    272.740   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        22949.000
 0.000000000D+00 0.000000000D+00 1.074386830D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00              -2.578789850D+04-4.803221290D+01
IRFNA            Wt%: HNO3(L) 83.5; N2O4(L) 14.; H2O(L) 2.; HF(g) .5.
 0 g 4/95 H   1.57N   1.63O   4.70F   0.02    0.00 1  100.0000000    -270496.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
JP-4             Or RP-1(L). NASA RP-1311, Part II, 1996. Hcomb = 18640.BTU/#
 0 g 5/95 C   1.00H   1.94    0.00    0.00    0.00 1   13.9687200     -22723.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
JP-5             Or ASTMA1(L). NASA RP-1311, Part II, 1996. Hcomb = 18600.BTU/#
 0 g 5/95 C   1.00H   1.92    0.00    0.00    0.00 1   13.9447300     -22183.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
Jet-A(L)         NASA TM-101475,1988. Hcomb=18500 BTU/#:NASA CR-72951,1971.
 1 g 2/96 C  12.00H  23.00    0.00    0.00    0.00 1  167.3110200    -303403.000
    220.000    550.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-4.218467340D+05-5.576234840D+03 1.522094335D+02-8.610096140D-01 3.071640926D-03
-4.702766120D-06 2.743009309D-09              -3.238535350D+04-6.780954740D+02
Jet-A(g)         NASA TM-101475,1988. NASA CR-72951,1971.
 2 g 2/96 C  12.00H  23.00    0.00    0.00    0.00 0  167.3110200    -249657.000
    273.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
-6.068699280D+05 8.328264220D+03-4.312323550D+01 2.572391032D-01-2.629316827D-04
 1.644989491D-07-4.645336690D-11              -7.606965040D+04 2.794306583D+02
   1000.000   5000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 1.541871660D+07-7.433869020D+04 1.468645380D+02-1.297042936D-02 2.159140196D-06
-1.887183642D-10 6.604559540D-15              3.996323340D+05-9.266675306D+02
LiCLO4(s)        Lithium Perchlorate. JANAF, March, 1964.
 0 j 3/64 LI  1.00CL  1.00O   4.00    0.00    0.00 1  106.3913000    -380700.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
NF3(L)           Nitrogen trifluoride. JANAF Prop.Ser.E,1/67.
 0 g 3/95 N   1.00F   3.00    0.00    0.00    0.00 1   71.0019500    -150387.000
    144.090      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
NH3(L)           Ammonia. TRC m-500,6/56,B.P.a-500,12/63. JANAF Prop.Ser.E,1/67
 0 g 3/95 N   1.00H   3.00    0.00    0.00    0.00 1   17.0305600     -71555.000
    239.720      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
NH4CLO4(I)       Ammonium Perchlorate. JANAF Dec.1962.
 1 j12/62 N   1.00H   4.00CL  1.00O   4.00    0.00 1  117.4888000    -295767.000
    100.000    513.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25238.000
-3.075345570D+03-2.136505940D+02 1.021583070D+01 1.659463750D-02 1.665266420D-05
-2.306096050D-08 1.543657320D-11              -3.825767260D+04-4.230254270D+01
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NH4CLO4(II)      Ammonium Perchlorate. JANAF Dec.1962.
 1 j12/62 N   1.00H   4.00CL  1.00O   4.00    0.00 2  117.4888000    -295767.000
    513.150   1500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        25238.000
 4.296999480D+07-3.178417800D+05 9.591437550D+02-1.439881370D+00 1.222673650D-03
-5.215401620D-07 8.803612760D-11                1.687446300D+06-5.889478160D+03
NH4NO3(IV)       Ammonium Nitrate Rhombic Crystal(IV). TPIS,1989.
 2 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 1   80.0434400    -365600.000
    256.200    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
-1.626679000D+07 2.614603390D+05-1.680046300D+03 5.448971540D+00-8.587849850D-03
 5.343277780D-06 0.000000000D+00               -1.264195170D+06 9.085696170D+03
    298.150    305.3807 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 5.865649330D+00 3.643028870D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.733937230D+04-2.614362440D+01
NH4NO3(III)      Ammonium Nitrate Rhombic Crystal(III). TPIS,1989.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 3   80.0434400    -365600.000
    305.380    357.2507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 7.233138210D+00 2.333270390D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.694179380D+04-2.929851690D+01
NH4NO3(II)       Ammonium Nitrate Tetragonal Crystal(II). TPIS,1989.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 4   80.0434400    -365600.000
    357.250    399.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 6.023205220D+01-1.767993540D-01 0.000000000D+00
 4.528829720D-07 0.000000000D+00               -5.478633510D+04-2.757806210D+02
NH4NO3(I)        Ammonium Nitrate Cubic Crystal(I). TPIS,1989.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 5   80.0434400    -365600.000
    399.000    442.8507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 1.295325880D+01 1.563531710D-02 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.783701280D+04-5.848510820D+01
NH4NO3(L)        Ammonium Nitrate Liquid. TPIS,1989.
 1 tpis89 N   2.00H   4.00O   3.00    0.00    0.00 6   80.0434400    -365600.000
    442.850   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        23662.000
 0.000000000D+00 0.000000000D+00 1.936373880D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.843793300D+04-8.903005280D+01
N2(L)            Nitrogen. TRC k-460,6/60, m-470,6/56. JANAF Prop.Ser.D,3/66.
 0 g 4/95 N   2.00    0.00    0.00    0.00    0.00 1   28.0134800     -12107.000
     77.352      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
N2H4(L)          Hydrazine. Hf298: TPIS89. Props: JANAF 12/65.
 1 j12/65 N   2.00H   4.00    0.00    0.00    0.00 1   32.0452400      50380.000
    100.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0           0.000
 2.080965740D+04-7.418167700D+02 1.916569190D+01-4.539330140D-02 1.342024260D-04
-1.470873940D-07 6.056288280D-11                5.735408210D+03-8.820213970D+01
N2O4(L)          Dinitrogen tetroxide. Hvap: JANAF Prop.Ser.C,4/65.
 0 g 4/95 N   2.00O   4.00    0.00    0.00    0.00 1   92.0110800     -17549.000
    298.150      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
O2(L)            Oxygen. Hvap: TRC m-10,12/63. JANAF Prop.Ser.D,3/66.
 0 g 4/95 O   2.00    0.00    0.00    0.00    0.00 1   31.9988000     -12979.000
     90.170      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
O3(L)            Ozone. Hvap: TRC m-10,12/63. JANAF Prop.Ser.E,1/67.
 0 g 4/95 O   3.00    0.00    0.00    0.00    0.00 1   47.9982000     122527.000
    161.850      0.0000  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0           0.000
RP-1 Mehta et.al. AIAA 95-2962 1995. Hcomb(high) = 19923.BTU/#
0 gll/00 C 1.00H 1.95 0.00 0.00 0.00 1 13.9761830 -24717.700
298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.000
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