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CAP: A Computer Code for Generating Tabular Thermodynamic Functions from NASA Lewis Coefficients

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February 2002

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Document Change History

This printing, numbered as **NASA/TM—2001-210959/REV1, February 2002,** replaces the previous version, **NASA/TM—2001-210959, October 2001**. It contains the following changes:

Page 2: Equation 3

$$S^o(T)/R = -a_1T^{-2}/2 - a_2T^{-1} + a_3\,(lnT) + a_4T + a_5T^2/2 + a_6T^3/3 + a_7T^4/4 + b_2 \quad (3)$$

Page 57: Table IC, record 2, the Fortran format molecular weight is F13.7

Page 57: Table IC, record 2, the Fortran format heat of formation at 298.15 K, J/mol is F15.5

Note that at the time of research, the NASA Lewis Research Center was undergoing a name change to the NASA John H. Glenn Research Center at Lewis Field. Both names may appear in this report.

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Introduction

For several decades the NASA Glenn Research Center has been providing a file of thermodynamic data for use in several computer programs (Gordon and McBride, 1994; McBride and Gordon, 1996; and Radhakrishnan and Bittker, 1994). These data are in the form of least-squares coefficients that have been calculated from tabular thermodynamic data by means of the NASA Properties and Coefficients (PAC) program (McBride and Gordon, 1992). The source thermodynamic data are obtained from the literature or from standard compilations (e.g., Chase, 1998; Gurvich et al., 1989, 1991, 1996; Barin, 1989; and TRC Thermodynamic Tables). Most gas-phase thermodynamic functions are calculated by the authors from molecular constant data using ideal gas partition functions.

The Coefficients and Properties (CAP) program described in this report permits the generation of tabulated thermodynamic functions from the NASA least-squares coefficients. CAP provides considerable flexibility in the output format, the number of temperatures to be tabulated, and the energy units of the calculated properties. This report provides a detailed description of input preparation, examples of input and output for several species, and a listing of all species in the current NASA Glenn thermodynamic data file.

Symbols

a_i (i = 1,7)	temperature coefficients in eqs. (1), (2), and (3)
b_1,b_2	integration constants defined by eqs. (2) and (3)
$C_p^o(T)$	molar heat capacity at constant pressure at temperature for standard state
$G^o(T)$	either $[G^o(T) - H^o(0)] + H^o(0)$ or $[G^o(T) - H^o(298.15)] + H^o(298.15)$
$G^o(T) - H^o(0)$	molar Gibbs energy at temperature T relative to enthalpy at 0 K for standard state
$G^o(T) - H^o(298.15)$	molar Gibbs energy at temperature T relative to enthalpy at 298.15 K for standard state
$\Delta_f G^o(T)$	molar Gibbs energy of formation of a substance at temperature T from its reference elements in their standard states
$H^o(0)$	chemical energy (molar enthalpy) at 0 K for standard state
$H^o(298.15)$	assigned molar enthalpy at 298.15 K for standard state (equals $\Delta_f H^o(298.15)$)
$H^o(T)$	either $[H^o(T) - H^o(0)] + H^o(0)$ or $[H^o(T) - H^o(298.15)] + H^o(298.15)$
$H^o(T) - H^o(0)$	molar enthalpy at temperature T relative to molar enthalpy at 0 K for standard state
$H^o(T) - H^o(298.15)$	molar enthalpy at temperature T relative to molar enthalpy at 298.15 K for standard state
$\Delta_f H^o(T)$	molar enthalpy of formation (heat of formation) of a substance at temperature T from its reference elements in their standard state
K	equilibrium constant
M	molecular weight
m_e	electron mass 0.0005485799039(13) amu
R	universal gas constant, 8.314510 J/(mol-K)
$S^o(T)$	entropy at temperature T for standard state
T	temperature, K

Background

The NASA Glenn equilibrium computer program, Chemical Equilibrium with Applications (CEA), is the latest in a series of thermodynamics tools generated at NASA Glenn Research Center to apply equilibrium thermodynamics to practical problems (Gordon and McBride, 1994; and McBride and Gordon, 1996). The core of these

programs is rapid solution of the equations that derive from free-energy minimization of multicomponent chemical systems at equilibrium. These programs require thermodynamic data for all species involved in their calculations. For easy input, CEA uses a 9-constant representation of the thermodynamic data. In this representation, $C_p^o(T)/R$ is expressed as a 7-coefficient power series in T (in Kelvin), with integration constants b_1 for $H^o(T)/RT$ and b_2 for $S^o(T)/R$:

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

$$H^o(T)/RT = -a_1T^{-2} + a_2(lnT)/T + a_3 + a_4T/2 + a_5T^2/3 + a_6T^3/4 + a_7T^4/5 + b_1/T \quad (2)$$

$$S^o(T)/R = -a_1T^{-2}/2 - a_2T^{-1} + a_3(lnT) + a_4T + a_5T^2/2 + a_6T^3/3 + a_7T^4/4 + b_2 \quad (3)$$

This 9-constant form has been used since 1994. It supersedes an earlier 7-constant form (McBride et al., 1993a).

NASA Glenn Research Center maintains a database with 9-constant empirical coefficients for over 2000 species. These coefficients were generated by least-squares fits to measured or calculated thermodynamic functions for condensed and gas-phase species (McBride and Gordon, 1992). The database is continually updated to reflect new species, improved measurements for current species, and newer physical constants. It is the purpose of CAP to generate thermodynamic functions in tabular form from the NASA coefficient database.

The empirical coefficients in the NASA Glenn database have been generated through simultaneous least-squares fitting of $C_p^o(T)/R$, $S^o(T)/R$, and $H^o(T)/RT$ over temperature segments specific to the species (Zeleznik and Gordon, 1961). For solid phases, this temperature range corresponds to the range in which the phase is stable at 10^5 Pa (1 bar). Liquids are generally fit from the melting point to 6000 K. The fitted temperature range for solids and gases starts at 200 K, but for ions it starts at 298.15 K. The range ends at 20 000 K for monatomic gases and some simple molecules. The range ends at 6000 K for most polyatomic molecules.

Appendix A, page 5, lists the individual species contained in the database, the temperature ranges for which their coefficients are valid, $\Delta_f H^o(298.15)$ for each species, and a reference code identifying the date and source of the latest update of that species. The list is arranged in the same order as the database: first gas-phase species, followed by condensed species, and then species that are used as reactants only. It is also important to note that in the "NAME" column, all letters "L" are capitalized to distinguish them from the number one, e.g., "CL," "AL," and "Ba(L)." The NASA reference codes (e.g., tpis96) are explained in a footnote to appendix A.

Reference States and Reference Elements

For the NASA Glenn database, the reference state for every element has been chosen to be the stable phase of the pure element at 298.15 K and 10^5 Pa (1 bar). The enthalpy of each element is assigned to be zero at this temperature and pressure. The enthalpy at 298.15 K and 10^5 Pa of any general compound of stoichiometry $A_xB_y \ldots C_z$ is defined to be the negative of the energy released when the compound forms from the elements in their reference states:

$$xA + yB + \ldots + zC = A_xB_y \ldots C_z;\ H^o(298.15) \equiv \Delta_f H^o(298.15) = -\Delta H_{rxn} \quad (4)$$

This relationship defines the contribution of each element to the compound's enthalpy at 298.15 K. For temperatures other than 298.15 K, the enthalpy equals the sum of the heat of formation at 298.15 K and any sensible heat:

$$H^o(T) = \Delta_f H^o(298.15) + [H^o(T) - H^o(298.15)] \quad (5)$$

where $[H^o(T) - H^o(298.15)]$ includes the enthalpies of phase changes as well as $\int_{298.15}^{T} C_p^o(T)dT$ contributions.

NASA TP–3287 (McBride et al., 1993b) is a compilation of the thermodynamic functions $C_p^o(T)$, $[H^o(T) - H^o(0)]$, $S^o(T)$, $-[G^o(T) - H^o(0)]/T$, $H^o(T)$, and $-G^o(T)/T$ for 50 elements in their standard states. These reference elements are listed in appendix B, page 45. It is to be noted that some of the data in NASA TP–3287 have been revised since publication: (1) Ga(cr,l) and In(cr,l) have been added (Gurvich et al., 1996); (2) Sc(α,β,l) has been added (Gurvich et al., 1982); and (3) the noble gases (He, Ne, Ar, Kr, and Xe) have been revised and Rn has been added (Gordon and McBride, 1999).

Properties and Coefficients (PAC) Programs

Most of the coefficients in the NASA Glenn database were generated with the NASA Properties and Coefficients (PAC) programs. The PAC series (PAC1, PAC5, PAC91, and PAC99) are FORTRAN programs that generate theoretical thermodynamic functions from molecular constant data and enable fitting these functions to empirical

equations by means of a least-squares fit. The PAC programs are quite flexible and allow a wide range of options for the least-squares fit: $C_p^o(T)/R$ only; simultaneous fits of $C_p^o(T)/R$, $H^o(T)/RT$, and $S^o(T)/R$; and a range of choices in the number of terms and exponents to T.

A full discussion of the PAC91 program is contained in McBride and Gordon (1992). The current version is PAC99, containing updated physical constants (Cohen, 1987), atomic weights (Coplen, 1996), and several new options for calculating monatomic atom partition functions (Gordon and McBride, 1999).

Since most of the coefficients in the NASA Glenn database were generated using PAC, it is useful to discuss the least-squares parameters used by PAC and the format of the coefficient files it generates. The user provides PAC with either the data that allow the program to generate the thermodynamic functions to be fitted, or tabulated values of these functions. These data will be, for example, molecular data and spectroscopic term values for gases, or T versus $C_p^o(T)$, $S^o(T)$, and $[H^o(T) - H^o(0)]$ values for gases or condensed species. These data must span the temperature range to be fitted. PAC uses the least-squares method to fit the data, subject to certain constraints: (a) $C_p^o(T)/R$ is fit to equation (1); (b) For gases, the temperature range is split into three intervals: 200 to 1000 K (298.15 to 1000 K for ions), 1000 to 6000 K, and 6000 to 20 000 K; (c) a fitting constraint requires an exact fit at 298.15 K; (d) another fitting constraint requires coefficients in any two contiguous intervals to yield the same values of the functions at the common temperature, except for phase transitions, where only the values of $\Delta_f G^o(T)$ are equal; and (e) generally, the functions $C_p^o(T)/R$, $[H^o(T) - H^o(0)]/R$, and $S^o(T)/R$ are fit simultaneously. For condensed species, each phase has its own set of coefficients. PAC performs the least-squares fit and prints out a file containing the coefficients a_1 through a_7, b_1, and b_2 in a format acceptable to the CAP and CEA programs. This format is described in appendix C, page 57.

Use of the CAP Program

This section will describe the form and format of the input necessary for use of the CAP program. Sample problems and examples in appendix D will clarify the discussion.

The following definitions will be used in this section:

- The "standard state" for a gaseous species is defined as its state at the standard pressure of 10^5 Pa (1 bar). For condensed species, the standard state is the pure crystalline or liquid substance at the same standard pressure.
- The term "log K" indicates the logarithm to the base 10 of the equilibrium constant that would result in the formation of a species from the elements in their standard states. This quantity equals $-\Delta_f G^o(T)/(2.30325851RT)$ for the species.

CAP requires only one input file. This file specifies output parameters, a temperature schedule, and coefficient sets for all species to be processed. In addition, if log K and $\Delta_f H^o(T)$ values are desired, a second file must be present containing enthalpies and entropies for all elements contained in all species. CAP expects this reference file, named "cap.elms," to be present in the working directory. The cap.elms file is discussed on page 45, appendix B.

To use CAP, the user first compiles the source code with a FORTRAN compiler to generate an executable file (to be named "cap.x" for the present discussion). The user prepares an input file (e.g., "cap.input") according to the rules discussed below, and uses standard redirection to generate the output:

cap.x < cap.input > cap.output

The CAP Input File

An example of a CAP input file is shown in appendix D, page 59. The input file consists of two records, called the keyword record and the temperature record, followed by coefficient records for each species to be listed.

Keyword Record.—Record 1 (keyword record) of the CAP input file contains a list of keywords describing the format to be used in the output tables. These keywords can be all uppercase or lowercase and listed in any order. Any number of allowable keywords can be included in this record. The format is

'kw_1', 'kw_2', 'kw_3', 'kw_4', . . . 'kw_{end}'/

Each keyword must be enclosed in quotes. The keywords must be separated by one or more spaces or commas. The record must end with a slash.

The seven possible keywords are as follows:

JOULES	output energy units in joules/mole and kilojoules/mole
CAL	output energy units in calories/mole and kilocalories/mole
ENGR	output units in "engineering" units (British thermal units per pound (BTU/lb) and British thermal units per pound-degree Rankine (BTU/lb-°R). If this keyword is specified, the input temperature schedule (see next section) must be specified in degrees Rankine. This keyword supersedes JOULES or CAL.)

MFIG thermodynamic functions $C_p^o(T)$, $H^o(T)–H^o(0)$, $S^o(T)$, $–[G^o(T)–H^o(0)]$, $H^o(T)$, and $–G^o(T)$, printed with five to seven places after the decimal (No $\Delta_f H^o(T)$ or log K values are to be printed.)

LOGK $\Delta_f H^o(T)$ and log K values are printed along with the thermodynamic functions $C_p^o(T)$, $[H^o(T)–H^o(298.15)]$, $S^o(T)$, $H^o(T)$, and $[G^o(T)–H^o(298.15)]$ (This table is rounded to three or four decimal places.)

NODIM dimensionless output (thermodynamic functions are divided by R or RT, printed with five to seven places after the decimal.)

PLOT A file named "plotout" is created containing T (in degrees Kelvin), $C_p^o(T)/R$, $[H^o(T)–H^o(0)]/RT$, $S^o(T)/R$, $–[G^o(T)–H^o(T)]/RT$, $H^o(T)/RT$ and $–G^o(T)/RT$, in columns (If $[H^o(298.15)–H^o(0)]$ has not been supplied, plotout contains $[H^o(T)–H^o(298.15)]/RT$ instead of $[H^o(T)–H^o(0)]/RT$.)

All temperatures in the plotout file are in degrees Kelvin.

These keywords may appear in any order in the keyword record. If mutually exclusive keywords are specified, separate tables are printed.

Temperature Record.—Record 2 (temperature record) of the CAP input file contains the temperature schedule desired, in the form of temperatures and temperature intervals. All species for the current run will use this temperature schedule. The format for the temperature record is as follows:

$$T_1, int_1, T_2, int_2, T_3, int_3, T_4, \ldots, T_{end}/$$

where the int_n values specify the temperature interval to be used between temperatures T_n and T_{n+1}. Temperatures must be in degrees Kelvin unless the keyword ENGR has been specified, in which case the temperatures must be in degrees Rankine. The sign of int_n must be consistent with that of $(T_{n+1} – T_n)$. These temperatures are separated by one or more spaces or commas, and the line must be terminated with a slash. A zero value for int_n, or two adjacent commas, tells CAP to proceed to the next temperature. CAP automatically inserts endpoints, 298.15 K, and phase transition points if within the requested range. For phase transition points, the output listing contains data for both phases. The program allows up to 500 temperatures per species.

Coefficients Records.—All records in the input file following the first two must contain thermodynamic coefficients for all species to be processed by CAP. These coefficients will usually be copied from the NASA Glenn database. CAP will generate output tables for each species whose coefficients are provided. An unlimited number of species may be run. For species with several phases, the phases must be supplied in increasing order by temperature. If the temperature range spanned by the coefficients is exceeded by the temperature schedule in record 2, CAP uses the coefficients for a range up to 20 percent beyond the endpoint. Examples 1 to 5 in appendix D clarify these points.

The Reference Element File (cap.elms)

To calculate $\Delta_f H^o(T)$ and log K values for any chemical species, CAP requires enthalpies and free energies for the elements that comprise that species. This information must be present in a reference file accessible to the program. The cap.elms file, which is distributed with the program, contains this information for many elements plus the electron gas, in the standard 9-constant NASA coefficient form. If an element is not included in cap.elms, log K and $\Delta_f H^o(T)$ values will not be printed for compounds containing that element. In addition, log K and $\Delta_f H^o(T)$ tables will not contain any values above or below the range covered in cap.elms for the elements comprising that species. Appendix B, page 45, lists the contents of the cap.elms file as of the date of this report.

Appendix A
Individual Species Contained in the NASA Glenn Thermochemical Database

ORDER OF SPECIES:
1) Gaseous products/reactants (numbers 1-1250)
2) Condensed products/reactants (numbers 1251-2015)
3) Gaseous/condensed reactants only (numbers 2016-2038)

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^\circ(298.15)$
1	e-	g12/98	298.15 - 20000.00	0.000
2	Ag	g10/97	200.00 - 20000.00	284.900
3	Ag+	g10/97	298.15 - 20000.00	1022.094
4	Ag-	g10/97	298.15 - 20000.00	153.079
5	AL	g12/97	200.00 - 20000.00	330.000
6	AL+	g 1/98	298.15 - 20000.00	913.015
7	AL-	g 3/97	298.15 - 20000.00	281.090
8	ALBr	tpis96	200.00 - 6000.00	14.325
9	ALBr2	tpis96	200.00 - 6000.00	-140.662
10	ALBr3	tpis96	200.00 - 6000.00	-410.477
11	ALC	tpis96	200.00 - 6000.00	682.284
12	ALC2	tpis96	200.00 - 6000.00	675.616
13	ALCL	tpis96	200.00 - 6000.00	-51.007
14	ALCL+	j 6/76	298.15 - 6000.00	861.849
15	ALCL2	tpis96	200.00 - 6000.00	-240.874
16	ALCL3	tpis96	200.00 - 6000.00	-584.679
17	ALF	tpis96	200.00 - 6000.00	-264.060
18	ALF+	j 6/76	298.15 - 6000.00	692.234
19	ALFCL	tpis96	200.00 - 6000.00	-436.410
20	ALFCL2	tpis96	200.00 - 6000.00	-791.395
21	ALF2	tpis96	200.00 - 6000.00	-631.764
22	ALF2-	tpis96	298.15 - 6000.00	-853.231
23	ALF2CL	tpis96	200.00 - 6000.00	-999.128
24	ALF3	tpis96	200.00 - 6000.00	-1209.277
25	ALF4-	tpis96	298.15 - 6000.00	-1951.601
26	ALH	tpis96	200.00 - 6000.00	249.251
27	ALHCL	tpis96	200.00 - 6000.00	10.522
28	ALHCL2	tpis96	200.00 - 6000.00	-351.279
29	ALHF	tpis96	200.00 - 6000.00	-182.614
30	ALHFCL	tpis96	200.00 - 6000.00	-555.245
31	ALHF2	tpis96	200.00 - 6000.00	-765.299
32	ALH2	tpis96	200.00 - 6000.00	276.775
33	ALH2CL	tpis96	200.00 - 6000.00	-106.345
34	ALH2F	tpis96	200.00 - 6000.00	-316.656
35	ALH3	tpis96	200.00 - 6000.00	128.896
36	ALI	tpis96	200.00 - 6000.00	67.395
37	ALI2	tpis96	200.00 - 6000.00	-33.813
38	ALI3	tpis96	200.00 - 6000.00	-191.330
39	ALN	tpis96	200.00 - 6000.00	438.829
40	ALO	tpis96	200.00 - 20000.00	67.319
41	ALO+	j12/79	298.15 - 6000.00	992.993
42	ALO-	g11/97	298.15 - 6000.00	-272.922
43	ALOCL	tpis96	200.00 - 6000.00	-301.565

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
44	ALOCL2	tpis96	200.00 - 6000.00	-402.309
45	ALOF	tpis96	200.00 - 6000.00	-572.290
46	ALOF2	tpis96	200.00 - 6000.00	-773.650
47	ALOF2-	g 2/01	298.15 - 6000.00	-972.290
48	ALOH	tpis96	200.00 - 6000.00	-192.762
49	ALOHCL	tpis96	200.00 - 6000.00	-373.786
50	ALOHCL2	tpis96	200.00 - 6000.00	-725.145
51	ALOHF	tpis96	200.00 - 6000.00	-574.212
52	ALOHF2	tpis96	200.00 - 6000.00	-1141.511
53	ALO2	tpis96	200.00 - 6000.00	-38.658
54	ALO2-	tpis96	298.15 - 6000.00	-452.572
55	AL(OH)2	tpis96	200.00 - 6000.00	-507.661
56	AL(OH)2CL	tpis96	200.00 - 6000.00	-859.057
57	AL(OH)2F	tpis96	200.00 - 6000.00	-1069.629
58	AL(OH)3	tpis96	200.00 - 6000.00	-1012.668
59	ALS	tpis96	200.00 - 6000.00	232.682
60	ALS2	tpis96	200.00 - 6000.00	248.535
61	AL2	tpis96	200.00 - 6000.00	501.302
62	AL2Br6	tpis96	200.00 - 6000.00	-942.423
63	AL2C2	tpis96	200.00 - 6000.00	544.978
64	AL2CL6	tpis96	200.00 - 6000.00	-1296.876
65	AL2F6	tpis96	200.00 - 6000.00	-2632.491
66	AL2I6	tpis96	200.00 - 6000.00	-487.747
67	AL2O	tpis96	200.00 - 6000.00	-148.611
68	AL2O+	g 1/01	298.15 - 6000.00	648.970
69	AL2O2	tpis96	200.00 - 6000.00	-403.096
70	AL2O2+	g 2/01	298.15 - 6000.00	557.439
71	AL2O3	tpis96	200.00 - 6000.00	-546.891
72	AL2S	tpis96	200.00 - 6000.00	220.679
73	AL2S2	tpis96	200.00 - 6000.00	135.287
74	Ar	g 3/98	200.00 - 20000.00	0.000
75	Ar+	g 1/99	298.15 - 20000.00	1526.778
76	B	g 9/98	200.00 - 20000.00	575.599
77	B+	g 9/98	298.15 - 20000.00	1382.316
78	B-	g 9/98	298.15 - 20000.00	542.631
79	BBr	g 9/98	200.00 - 6000.00	240.952
80	BBr2	g 9/98	200.00 - 6000.00	97.829
81	BBr3	tpis96	200.00 - 6000.00	-205.300
82	BC	g 9/98	200.00 - 6000.00	838.162
83	BC2	g 9/98	200.00 - 6000.00	801.259
84	BCL	g 9/98	200.00 - 6000.00	183.173
85	BCL+	j 6/68	298.15 - 6000.00	1234.280
86	BCLOH	g 9/98	200.00 - 6000.00	-234.005
87	BCL(OH)2	tpis96	200.00 - 6000.00	-805.388
88	BCL2	tpis96	200.00 - 6000.00	-60.881
89	BCL2+	g 1/01	298.15 - 6000.00	672.315
90	BCL2OH	tpis96	200.00 - 6000.00	-604.917
91	BCL3	tpis96	200.00 - 6000.00	-404.500
92	BF	g10/97	200.00 - 6000.00	-106.932
93	BFCL	tpis96	200.00 - 6000.00	-279.184
94	BFCL2	tpis96	200.00 - 6000.00	-643.000
95	BFOH	g 9/98	200.00 - 6000.00	-451.632
96	BF(OH)2	tpis96	200.00 - 6000.00	-1049.890
97	BF2	tpis96	200.00 - 6000.00	-499.427

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
98	BF2+	j12/70	298.15 - 6000.00	322.586
99	BF2-	tpis96	298.15 - 6000.00	-733.803
100	BF2CL	tpis96	200.00 - 6000.00	-888.000
101	BF2OH	tpis96	200.00 - 6000.00	-1092.217
102	BF3	tpis96	200.00 - 6000.00	-1136.000
103	BF4-	tpis96	298.15 - 6000.00	-1761.266
104	BH	g12/99	200.00 - 6000.00	448.727
105	BHCL	g 9/98	200.00 - 6000.00	141.418
106	BHCL2	tpis96	200.00 - 6000.00	-251.884
107	BHF	g 9/98	200.00 - 6000.00	-76.012
108	BHFCL	tpis96	200.00 - 6000.00	-483.037
109	BHF2	tpis96	200.00 - 6000.00	-739.614
110	BH2	g 2/00	200.00 - 6000.00	328.909
111	BH2CL	tpis96	200.00 - 6000.00	-80.846
112	BH2F	tpis96	200.00 - 6000.00	-323.957
113	BH3	g 1/00	200.00 - 6000.00	104.747
114	BH3NH3	tpis96	200.00 - 6000.00	-115.000
115	BH4	g 5/00	200.00 - 6000.00	255.210
116	BH5	g 8/00	200.00 - 6000.00	92.934
117	BI	g 9/98	200.00 - 6000.00	325.988
118	BI2	g 9/98	200.00 - 6000.00	238.096
119	BI3	tpis96	200.00 - 6000.00	21.400
120	BN	g 9/98	200.00 - 6000.00	574.726
121	BO	g 9/98	200.00 - 20000.00	20.406
122	BO-	g 9/98	298.15 - 6000.00	-277.791
123	BOCL	tpis96	200.00 - 6000.00	-318.537
124	BOCL2	tpis96	200.00 - 6000.00	-361.566
125	BOF	tpis96	200.00 - 6000.00	-592.978
126	BOF2	tpis96	200.00 - 6000.00	-832.768
127	BOH	tpis96	200.00 - 6000.00	-6.757
128	BO2	g10/97	200.00 - 6000.00	-309.122
129	BO2-	tpis96	298.15 - 6000.00	-714.494
130	B(OH)2	g 9/98	200.00 - 6000.00	-425.244
131	BS	g10/98	200.00 - 6000.00	273.519
132	BS2	g 9/98	200.00 - 6000.00	63.867
133	B2	g 9/98	200.00 - 6000.00	857.371
134	B2C	g 9/98	200.00 - 6000.00	800.433
135	B2CL4	g10/97	200.00 - 6000.00	-490.000
136	B2F4	g10/97	200.00 - 6000.00	-1438.000
137	B2H	g 7/00	200.00 - 6000.00	796.262
138	B2H2	g 7/00	200.00 - 6000.00	454.678
139	B2H3	g 6/00	200.00 - 6000.00	351.073
140	B2H3,db	g 7/00	200.00 - 6000.00	353.408
141	B2H4	g 8/00	200.00 - 6000.00	211.162
142	B2H4,db	g 7/00	200.00 - 6000.00	209.932
143	B2H5	g 5/00	200.00 - 6000.00	254.784
144	B2H5,db	g 5/00	200.00 - 6000.00	275.151
145	B2H6	g 5/00	200.00 - 6000.00	36.600
146	B2O	g 9/98	200.00 - 6000.00	192.798
147	B2O2	tpis96	200.00 - 6000.00	-457.711
148	B2O3	tpis96	200.00 - 6000.00	-835.382
149	B2(OH)4	g 9/98	200.00 - 6000.00	-1254.988
150	B2S	g 9/98	200.00 - 6000.00	622.261
151	B2S2	tpis96	200.00 - 6000.00	138.317

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o$(298.15)
152	B2S3	tpis96	200.00 - 6000.00	17.754
153	B3H7,C2v	g 8/00	200.00 - 6000.00	176.019
154	B3H7,Cs	g 8/00	200.00 - 6000.00	159.318
155	B3H9	g 7/00	200.00 - 6000.00	138.909
156	B3N3H6	tpis96	200.00 - 6000.00	-512.000
157	B3O3CL3	tpis96	200.00 - 6000.00	-1635.982
158	B3O3FCL2	tpis96	200.00 - 6000.00	-1883.808
159	B3O3F2CL	tpis96	200.00 - 6000.00	-2132.817
160	B3O3F3	tpis96	200.00 - 6000.00	-2382.699
161	B4H4	g 8/00	200.00 - 6000.00	326.190
162	B4H10	g 5/00	200.00 - 6000.00	66.100
163	B4H12	g 5/00	200.00 - 6000.00	188.236
164	B5H9	g 6/00	200.00 - 6000.00	73.220
165	Ba	g10/97	200.00 - 20000.00	185.000
166	Ba+	g10/97	298.15 - 20000.00	694.050
167	BaBr	tpis96	200.00 - 6000.00	-75.325
168	BaBr2	tpis96	200.00 - 6000.00	-412.515
169	BaCL	tpis96	200.00 - 6000.00	-136.291
170	BaCL+	g12/97	298.15 - 6000.00	348.698
171	BaCL2	tpis96	200.00 - 6000.00	-499.301
172	BaF	tpis96	200.00 - 6000.00	-318.994
173	BaF+	g12/97	298.15 - 6000.00	134.063
174	BaF2	tpis96	200.00 - 6000.00	-812.003
175	BaH	tpis96	200.00 - 6000.00	209.535
176	BaI	tpis96	200.00 - 6000.00	-10.238
177	BaI2	tpis96	200.00 - 6000.00	-288.440
178	BaO	tpis96	200.00 - 20000.00	-117.948
179	BaO+	g11/98	298.15 - 20000.00	511.705
180	BaOH	tpis96	200.00 - 6000.00	-224.257
181	BaOH+	tpis96	298.15 - 6000.00	202.019
182	Ba(OH)2	tpis96	200.00 - 6000.00	-606.666
183	BaS	tpis96	200.00 - 6000.00	38.871
184	Ba2	tpis96	200.00 - 6000.00	355.964
185	Be	g11/97	200.00 - 20000.00	324.000
186	Be+	g 1/98	298.15 - 20000.00	1229.701
187	Be++	g 3/97	298.15 - 20000.00	2993.002
188	BeBr	tpis96	200.00 - 6000.00	132.446
189	BeBr2	tpis96	200.00 - 6000.00	-234.062
190	BeCL	tpis96	200.00 - 6000.00	56.693
191	BeCL2	tpis96	200.00 - 6000.00	-361.539
192	BeF	tpis96	200.00 - 6000.00	-170.625
193	BeF2	tpis96	200.00 - 6000.00	-796.588
194	BeH	tpis96	200.00 - 6000.00	342.252
195	BeH+	g 1/01	298.15 - 20000.00	1178.219
196	BeH2	g 4/01	200.00 - 6000.00	161.099
197	BeI	tpis96	200.00 - 6000.00	207.454
198	BeI2	tpis96	200.00 - 6000.00	-64.759
199	BeN	j 6/63	200.00 - 6000.00	427.000
200	BeO	tpis96	200.00 - 20000.00	128.940
201	BeOH	tpis96	200.00 - 6000.00	-99.718
202	BeOH+	j12/75	298.15 - 20000.00	759.984
203	Be(OH)2	tpis96	200.00 - 6000.00	-638.864
204	BeS	tpis96	200.00 - 6000.00	247.095
205	Be2	tpis96	200.00 - 6000.00	637.543

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
206	Be2CL4	tpis96	200.00 - 6000.00	-819.605
207	Be2F4	tpis96	200.00 - 6000.00	-1731.700
208	Be2O	tpis96	200.00 - 6000.00	-37.034
209	Be2OF2	j 6/66	200.00 - 6000.00	-1204.574
210	Be2O2	tpis96	200.00 - 6000.00	-411.635
211	Be3O3	tpis96	200.00 - 6000.00	-1023.721
212	Be4O4	tpis96	200.00 - 6000.00	-1649.295
213	Br	g 3/97	200.00 - 20000.00	111.870
214	Br+	g10/97	298.15 - 20000.00	1257.927
215	Br-	g10/97	298.15 - 20000.00	-219.000
216	BrCL	tpis89	200.00 - 6000.00	14.789
217	BrF	tpis89	200.00 - 6000.00	-58.851
218	BrF3	tpis89	200.00 - 6000.00	-255.600
219	BrF5	tpis89	200.00 - 6000.00	-428.800
220	BrO	j 3/96	200.00 - 6000.00	125.800
221	OBrO	j 3/96	200.00 - 6000.00	151.955
222	BrOO	j 3/96	200.00 - 6000.00	108.000
223	BrO3	j 3/96	200.00 - 6000.00	220.821
224	Br2	tpis89	200.00 - 6000.00	30.910
225	BrBrO	j 3/96	200.00 - 6000.00	168.000
226	BrOBr	j 3/96	200.00 - 6000.00	107.639
227	C	g 7/97	200.00 - 20000.00	716.680
228	C+	g 6/98	298.15 - 20000.00	1809.444
229	C-	g 3/98	298.15 - 20000.00	588.314
230	CBr	tpis91	200.00 - 6000.00	490.432
231	CBr2	tpis91	200.00 - 6000.00	336.623
232	CBr3	tpis91	200.00 - 6000.00	235.000
233	CBr4	g 8/99	200.00 - 6000.00	79.500
234	CCL	g 8/99	200.00 - 6000.00	432.611
235	CCLBr3	tpis91	200.00 - 6000.00	65.000
236	CCL2	g 8/99	200.00 - 6000.00	222.940
237	CCL2Br2	tpis91	200.00 - 6000.00	10.000
238	CCL3	n12/93	200.00 - 6000.00	71.128
239	CCL3Br	tpis91	200.00 - 6000.00	-43.000
240	CCL4	tpis91	200.00 - 6000.00	-95.600
241	CF	tpis91	200.00 - 6000.00	242.300
242	CF+	g12/99	298.15 - 6000.00	1145.564
243	CFBr3	tpis91	200.00 - 6000.00	-120.000
244	CFCL	g 9/99	200.00 - 6000.00	25.846
245	CFCLBr2	tpis91	200.00 - 6000.00	-175.000
246	CFCL2	tpis91	200.00 - 6000.00	-105.000
247	CFCL2Br	tpis91	200.00 - 6000.00	-235.000
248	CFCL3	g 7/99	200.00 - 6000.00	-283.700
249	CF2	g 9/99	200.00 - 6000.00	-186.600
250	CF2+	g 9/99	298.15 - 6000.00	949.341
251	CF2Br2	tpis91	200.00 - 6000.00	-380.000
252	CF2CL	tpis91	200.00 - 6000.00	-275.000
253	CF2CLBr	tpis91	200.00 - 6000.00	-435.000
254	CF2CL2	g 7/99	200.00 - 6000.00	-490.800
255	CF3	g 8/99	200.00 - 6000.00	-467.400
256	CF3+	g 9/99	298.15 - 6000.00	423.617
257	CF3Br	tpis91	200.00 - 6000.00	-648.800
258	CF3CL	g 7/99	200.00 - 6000.00	-704.200
259	CF4	g 7/99	200.00 - 6000.00	-933.120

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
260	CH	tpis79	200.00 - 20000.00	597.371
261	CH+	tpis91	298.15 - 20000.00	1630.571
262	CHBr3	g 8/99	200.00 - 6000.00	16.740
263	CHCL	g 9/99	200.00 - 6000.00	297.100
264	CHCLBr2	tpis91	200.00 - 6000.00	10.000
265	CHCL2	n12/93	200.00 - 6000.00	95.800
266	CHCL2Br	tpis91	200.00 - 6000.00	-45.000
267	CHCL3	g 7/99	200.00 - 6000.00	-102.700
268	CHF	g 8/99	200.00 - 6000.00	108.800
269	CHFBr2	tpis91	200.00 - 6000.00	-175.000
270	CHFCL	tpis91	200.00 - 6000.00	-83.145
271	CHFCLBr	tpis91	200.00 - 6000.00	-230.000
272	CHFCL2	g 7/99	200.00 - 6000.00	-284.900
273	CHF2	n 6/88	200.00 - 6000.00	-238.900
274	CHF2Br	tpis91	200.00 - 6000.00	-422.000
275	CHF2CL	g 7/99	200.00 - 6000.00	-482.800
276	CHF3	g 8/99	200.00 - 6000.00	-693.300
277	CHI3	g 8/99	200.00 - 6000.00	210.874
278	CH2	g 8/99	200.00 - 6000.00	388.800
279	CH2Br2	g 8/99	200.00 - 6000.00	-14.770
280	CH2CL	g12/99	200.00 - 6000.00	119.200
281	CH2CLBr	tpis91	200.00 - 6000.00	-45.000
282	CH2CL2	tpis91	200.00 - 6000.00	-95.000
283	CH2F	x 6/88	200.00 - 6000.00	-31.800
284	CH2FBr	tpis91	200.00 - 6000.00	-215.000
285	CH2FCL	g 7/99	200.00 - 6000.00	-265.700
286	CH2F2	g 8/99	200.00 - 6000.00	-452.300
287	CH2I2	g 8/99	200.00 - 6000.00	117.570
288	CH3	g 8/99	200.00 - 6000.00	146.900
289	CH3Br	g 8/99	200.00 - 6000.00	-37.740
290	CH3CL	tpis91	200.00 - 6000.00	-81.870
291	CH3F	g 8/99	200.00 - 6000.00	-237.700
292	CH3I	g 8/99	200.00 - 6000.00	13.765
293	CH2OH	g11/00	200.00 - 6000.00	-17.800
294	CH2OH+	g11/00	298.15 - 6000.00	716.400
295	CH3O	g 7/00	200.00 - 6000.00	13.000
296	CH4	g 8/99	200.00 - 6000.00	-74.600
297	CH3OH	g 7/00	200.00 - 6000.00	-200.940
298	CI	tpis91	200.00 - 6000.00	570.201
299	CI2	tpis91	200.00 - 6000.00	468.394
300	CI3	g 9/99	200.00 - 6000.00	405.984
301	CI4	g 8/99	200.00 - 6000.00	267.943
302	CN	g 8/99	200.00 - 20000.00	438.684
303	CN+	tpis91	298.15 - 20000.00	1798.891
304	CN-	tpis91	298.15 - 6000.00	63.885
305	CNN	g12/99	200.00 - 6000.00	633.484
306	CO	tpis79	200.00 - 20000.00	-110.535
307	CO+	tpis91	298.15 - 20000.00	1247.789
308	COCL	tpis91	200.00 - 6000.00	-16.000
309	COCL2	tpis91	200.00 - 6000.00	-219.500
310	COFCL	tpis91	200.00 - 6000.00	-429.493
311	COF2	tpis91	200.00 - 6000.00	-640.000
312	COHCL	tpis91	200.00 - 6000.00	-164.212
313	COHF	tpis91	200.00 - 6000.00	-374.590

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
314	COS	g 5/01	200.00 - 6000.00	-141.700
315	CO2	g 9/99	200.00 - 20000.00	-393.510
316	CO2+	g 9/99	298.15 - 20000.00	944.688
317	COOH	tpis91	200.00 - 6000.00	-213.000
318	CP	tpis91	200.00 - 6000.00	520.162
319	CS	g 7/99	200.00 - 6000.00	279.765
320	CS2	g 6/95	200.00 - 6000.00	116.700
321	C2	tpis91	200.00 - 20000.00	830.457
322	C2+	tpis91	298.15 - 20000.00	2004.776
323	C2-	tpis91	298.15 - 6000.00	480.767
324	C2CL	tpis91	200.00 - 6000.00	534.083
325	C2CL2	tpis91	200.00 - 6000.00	200.000
326	C2CL3	tpis91	200.00 - 6000.00	190.272
327	C2CL4	tpis91	200.00 - 6000.00	-11.000
328	C2CL6	tpis91	200.00 - 6000.00	-141.500
329	C2F	tpis91	200.00 - 6000.00	353.847
330	C2FCL	tpis91	200.00 - 6000.00	33.766
331	C2FCL3	tpis91	200.00 - 6000.00	-166.000
332	C2F2	tpis91	200.00 - 6000.00	-144.666
333	C2F2CL2	tpis91	200.00 - 6000.00	-337.837
334	C2F3	tpis91	200.00 - 6000.00	-228.181
335	C2F3CL	tpis91	200.00 - 6000.00	-515.200
336	C2F4	tpis91	200.00 - 6000.00	-659.500
337	C2F6	g12/99	200.00 - 6000.00	-1344.000
338	C2H	g 6/01	200.00 - 6000.00	566.200
339	C2HCL	tpis91	200.00 - 6000.00	212.857
340	C2HCL3	g12/99	200.00 - 6000.00	-19.100
341	C2HF	tpis91	200.00 - 6000.00	41.692
342	C2HFCL2	tpis91	200.00 - 6000.00	-168.648
343	C2HF2CL	tpis91	200.00 - 6000.00	-333.654
344	C2HF3	tpis91	200.00 - 6000.00	-491.000
345	C2H2,acetylene	g 1/91	200.00 - 6000.00	228.200
346	C2H2,vinylidene	g 5/01	200.00 - 6000.00	414.788
347	C2H2CL2	tpis91	200.00 - 6000.00	3.410
348	C2H2FCL	tpis91	200.00 - 6000.00	-165.082
349	C2H2F2	tpis91	200.00 - 6000.00	-336.400
350	CH2CO,ketene	g 7/00	200.00 - 6000.00	-47.700
351	C2H3,vinyl	g 7/01	200.00 - 6000.00	299.687
352	C2H3CL	tpis91	200.00 - 6000.00	23.000
353	C2H3F	tpis91	200.00 - 6000.00	-140.100
354	CH3CN	g 9/00	200.00 - 6000.00	66.430
355	CH3CO,acetyl	g 6/96	200.00 - 6000.00	-10.000
356	C2H4	g 1/00	200.00 - 6000.00	52.500
357	C2H4O,ethylen-o	g 8/88	200.00 - 6000.00	-52.635
358	CH3CHO,ethanal	g 8/88	200.00 - 6000.00	-166.190
359	CH3COOH	g 6/00	200.00 - 6000.00	-432.249
360	C2H5	g 7/00	200.00 - 6000.00	118.658
361	C2H5Br	n 6/79	200.00 - 6000.00	-63.600
362	C2H6	g 7/00	200.00 - 6000.00	-83.852
363	CH3N2CH3	g 8/88	200.00 - 6000.00	148.699
364	C2H5OH	g 8/88	200.00 - 6000.00	-234.950
365	CH3OCH3	g 7/00	200.00 - 6000.00	-184.110
366	CCN	g 7/00	200.00 - 6000.00	804.596
367	CNC	tpis91	200.00 - 6000.00	684.915

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
368	C2N2	tpis79	200.00 - 6000.00	309.100
369	C2O	g 8/00	200.00 - 6000.00	291.039
370	C3	tpis79	200.00 - 20000.00	839.949
371	C3H3,1-propynl	n 4/98	200.00 - 6000.00	450.000
372	C3H3,2-propynl	n 4/98	200.00 - 6000.00	331.800
373	C3H4,allene	g 2/00	200.00 - 6000.00	190.920
374	C3H4,propyne	g 1/00	200.00 - 6000.00	184.900
375	C3H4,cyclo-	g 5/90	200.00 - 6000.00	277.100
376	C3H5,allyl	g 3/01	200.00 - 6000.00	163.594
377	C3H6,propylene	g 2/00	200.00 - 6000.00	20.000
378	C3H6,cyclo-	g 1/00	200.00 - 6000.00	53.300
379	C3H6O,propylox	g 6/01	200.00 - 6000.00	-93.720
380	C3H6O,acetone	g 6/97	200.00 - 6000.00	-217.150
381	C3H6O,propanal	g 5/01	200.00 - 6000.00	-186.000
382	C3H7,n-propyl	g 7/01	200.00 - 6000.00	100.500
383	C3H7,i-propyl	g 9/85	200.00 - 6000.00	93.300
384	C3H8	g 2/00	200.00 - 6000.00	-104.680
385	C3H8O,1propanol	g 2/00	200.00 - 6000.00	-255.200
386	C3H8O,2propanol	g 2/00	200.00 - 6000.00	-272.700
387	C3O2	g 7/88	200.00 - 6000.00	-93.638
388	C4	g tpis	200.00 - 20000.00	1033.904
389	C4H2,butadiyne	g 7/01	200.00 - 6000.00	450.000
390	C4H4,1,3-cyclo-	g 8/00	200.00 - 6000.00	385.000
391	C4H6,butadiene	n10/92	200.00 - 6000.00	110.000
392	C4H6,1butyne	n10/93	200.00 - 6000.00	165.200
393	C4H6,2butyne	n10/93	200.00 - 6000.00	145.700
394	C4H6,cyclo-	g 8/00	200.00 - 6000.00	156.700
395	C4H8,1-butene	n 4/88	200.00 - 6000.00	-0.540
396	C4H8,cis2-buten	n 4/88	200.00 - 6000.00	-7.400
397	C4H8,tr2-butene	n 4/88	200.00 - 6000.00	-11.000
398	C4H8,isobutene	n 4/88	200.00 - 6000.00	-17.100
399	C4H8,cyclo-	g 8/00	200.00 - 6000.00	28.400
400	(CH3COOH)2	g10/00	200.00 - 6000.00	-929.015
401	C4H9,i-butyl	n10/84	200.00 - 6000.00	57.320
402	C4H9,n-butyl	n10/84	200.00 - 6000.00	66.530
403	C4H9,s-butyl	g 1/93	200.00 - 6000.00	71.000
404	C4H9,t-butyl	g 1/93	200.00 - 6000.00	51.700
405	C4H10,isobutane	g 8/00	200.00 - 6000.00	-134.990
406	C4H10,n-butane	g12/00	200.00 - 6000.00	-125.790
407	C4N2	g 6/01	200.00 - 6000.00	529.200
408	C5	g 8/00	200.00 - 20000.00	1050.924
409	C5H6,1,3cyclo-	g 5/90	200.00 - 6000.00	134.300
410	C5H8,cyclo-	g 1/93	200.00 - 6000.00	33.900
411	C5H10,1-pentene	n 4/87	200.00 - 6000.00	-21.280
412	C5H10,cyclo-	g 2/01	200.00 - 6000.00	-77.100
413	C5H11,pentyl	n10/84	200.00 - 6000.00	45.810
414	C5H11,t-pentyl	g 1/93	200.00 - 6000.00	32.600
415	C5H12,n-pentane	n10/85	200.00 - 6000.00	-146.760
416	C5H12,i-pentane	n10/85	200.00 - 6000.00	-153.700
417	CH3C(CH3)2CH3	n10/85	200.00 - 6000.00	-167.920
418	C6D5,phenyl	g 1/01	200.00 - 6000.00	315.740
419	C6D6	g 1/01	200.00 - 6000.00	58.157
420	C6H2	g 2/93	200.00 - 6000.00	670.000
421	C6H5,phenyl	g11/00	200.00 - 6000.00	337.200

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
422	C6H5O,phenoxy	g 8/00	200.00 - 6000.00	47.700
423	C6H6	g 8/00	200.00 - 6000.00	82.880
424	C6H5OH,phenol	g 8/00	200.00 - 6000.00	-96.399
425	C6H10,cyclo-	g 1/93	200.00 - 6000.00	-4.600
426	C6H12,1-hexene	n 4/87	200.00 - 6000.00	-41.950
427	C6H12,cyclo-	g 6/90	200.00 - 6000.00	-123.300
428	C6H13,n-hexyl	n10/83	200.00 - 6000.00	25.100
429	C6H14,n-hexane	g 6/01	200.00 - 6000.00	-166.920
430	C7H7,benzyl	g 7/01	200.00 - 6000.00	210.500
431	C7H8	g 1/93	200.00 - 6000.00	50.170
432	C7H8O,cresol-mx	g12/00	200.00 - 6000.00	-132.298
433	C7H14,1-heptene	n 4/87	200.00 - 6000.00	-62.760
434	C7H15,n-heptyl	n10/83	200.00 - 6000.00	4.390
435	C7H16,2-methylh	n10/85	200.00 - 6000.00	-194.600
436	C7H16,n-heptane	n10/85	200.00 - 6000.00	-187.780
437	C8H8,styrene	n 4/89	200.00 - 6000.00	148.300
438	C8H10,ethylbenz	n10/86	200.00 - 6000.00	29.920
439	C8H16,1-octene	n 4/87	200.00 - 6000.00	-83.590
440	C8H17,n-octyl	n10/83	200.00 - 6000.00	-16.320
441	C8H18,n-octane	n 4/85	200.00 - 6000.00	-208.750
442	C8H18,isooctane	n 4/85	200.00 - 6000.00	-224.010
443	C9H19,n-nonyl	n10/83	200.00 - 6000.00	-37.030
444	C10H8,naphthale	g 3/01	200.00 - 6000.00	150.580
445	C10H21,n-decyl	n10/83	200.00 - 6000.00	-57.740
446	C12H9,o-bipheny	g 8/00	200.00 - 6000.00	427.730
447	C12H10,biphenyl	g 8/00	200.00 - 6000.00	182.130
448	Ca	g 8/97	200.00 - 20000.00	177.800
449	Ca+	g 1/98	298.15 - 20000.00	773.828
450	CaBr	tpis96	200.00 - 6000.00	-24.869
451	CaBr2	tpis96	200.00 - 6000.00	-387.197
452	CaCL	tpis96	200.00 - 6000.00	-103.773
453	CaCL+	tpis96	298.15 - 6000.00	467.191
454	CaCL2	tpis96	200.00 - 6000.00	-485.243
455	CaF	tpis96	200.00 - 6000.00	-276.404
456	CaF+	tpis96	298.15 - 6000.00	260.665
457	CaF2	tpis96	200.00 - 6000.00	-790.828
458	CaH	tpis96	200.00 - 6000.00	229.409
459	CaI	tpis96	200.00 - 6000.00	12.183
460	CaI2	tpis96	200.00 - 6000.00	-259.320
461	CaO	tpis96	200.00 - 20000.00	38.005
462	CaO+	tpis96	298.15 - 20000.00	710.238
463	CaOH	tpis96	200.00 - 6000.00	-173.307
464	CaOH+	tpis96	298.15 - 6000.00	372.938
465	Ca(OH)2	tpis96	200.00 - 6000.00	-598.339
466	CaS	tpis96	200.00 - 6000.00	121.475
467	Ca2	tpis96	200.00 - 6000.00	341.765
468	Cd	g 7/97	200.00 - 20000.00	111.800
469	Cd+	g 7/97	298.15 - 20000.00	985.754
470	CL	g 7/97	200.00 - 20000.00	121.301
471	CL+	g 1/98	298.15 - 20000.00	1378.800
472	CL-	g 4/97	298.15 - 20000.00	-233.958
473	CLCN	g 6/95	200.00 - 6000.00	134.200
474	CLF	tpis89	200.00 - 6000.00	-55.701
475	CLF3	tpis89	200.00 - 6000.00	-164.600

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
476	CLF5	tpis89	200.00 - 6000.00	-238.000
477	CLO	tpis89	200.00 - 6000.00	101.621
478	CLO2	g 7/93	200.00 - 6000.00	105.000
479	CL2	tpis89	200.00 - 6000.00	0.000
480	CL2O	tpis89	200.00 - 6000.00	79.000
481	Co	g 7/97	200.00 - 20000.00	428.442
482	Co+	g 7/97	298.15 - 20000.00	1193.003
483	Co-	g 9/97	298.15 - 20000.00	358.414
484	Cr	g 7/97	200.00 - 20000.00	397.480
485	Cr+	g 7/97	298.15 - 20000.00	1056.547
486	Cr-	g10/97	298.15 - 20000.00	327.023
487	CrN	j12/73	200.00 - 6000.00	505.009
488	CrO	tpis82	200.00 - 20000.00	186.581
489	CrO2	tpis82	200.00 - 6000.00	-108.043
490	CrO3	tpis82	200.00 - 6000.00	-322.037
491	CrO3-	tpis82	298.15 - 6000.00	-632.851
492	Cs	g 7/97	200.00 - 20000.00	76.500
493	Cs+	g 1/98	298.15 - 20000.00	458.402
494	Cs-	g10/97	298.15 - 20000.00	24.797
495	CsBO2	tpis82	200.00 - 6000.00	-686.902
496	CsBr	tpis82	200.00 - 6000.00	-206.829
497	CsCL	tpis82	200.00 - 6000.00	-242.229
498	CsF	tpis82	200.00 - 6000.00	-364.215
499	CsH	tpis82	200.00 - 6000.00	115.950
500	CsI	tpis82	200.00 - 6000.00	-152.320
501	CsLi	tpis82	200.00 - 6000.00	162.146
502	CsNO2	tpis82	200.00 - 6000.00	-210.340
503	CsNO3	tpis82	200.00 - 6000.00	-318.486
504	CsNa	tpis82	200.00 - 6000.00	125.907
505	CsO	tpis82	200.00 - 6000.00	37.587
506	CsOH	g 9/97	200.00 - 6000.00	-256.000
507	CsRb	tpis82	200.00 - 6000.00	111.477
508	Cs2	tpis82	200.00 - 6000.00	109.404
509	Cs2Br2	tpis82	200.00 - 6000.00	-565.829
510	Cs2CO3	tpis82	200.00 - 6000.00	-806.448
511	Cs2CL2	tpis82	200.00 - 6000.00	-644.658
512	Cs2F2	tpis82	200.00 - 6000.00	-891.859
513	Cs2I2	tpis82	200.00 - 6000.00	-454.033
514	Cs2O	tpis82	200.00 - 6000.00	-142.855
515	Cs2O+	tpis82	298.15 - 6000.00	283.700
516	Cs2O2	tpis82	200.00 - 6000.00	-247.069
517	Cs2O2H2	g 9/97	200.00 - 6000.00	-653.000
518	Cs2SO4	g10/99	200.00 - 6000.00	-1117.652
519	Cu	g12/97	200.00 - 20000.00	337.400
520	Cu+	g 3/98	298.15 - 20000.00	1089.080
521	Cu-	g10/97	298.15 - 20000.00	212.719
522	CuCL	j 3/66	200.00 - 6000.00	91.090
523	CuF	j12/77	200.00 - 6000.00	-12.550
524	CuF2	j12/77	200.00 - 6000.00	-266.940
525	CuO	j12/77	200.00 - 6000.00	306.270
526	Cu2	j 9/66	200.00 - 6000.00	485.340
527	Cu3CL3	j 3/66	200.00 - 6000.00	-258.570
528	D	g 6/97	200.00 - 20000.00	221.720
529	D+	g 9/96	298.15 - 20000.00	1540.324

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
530	D-	g 8/96	298.15 - 20000.00	142.753
531	DBr	tpis89	200.00 - 6000.00	-37.036
532	DCL	tpis89	200.00 - 6000.00	-93.547
533	DF	tpis89	298.15 - 20000.00	-276.228
534	DOCL	g 1/01	200.00 - 6000.00	-79.539
535	DO2	tpis89	200.00 - 6000.00	6.487
536	DO2-	tpis89	298.15 - 6000.00	-104.796
537	D2	tpis89	200.00 - 20000.00	0.000
538	D2+	j 9/77	298.15 - 6000.00	1498.568
539	D2-	j 9/77	298.15 - 6000.00	235.161
540	D2O	g 6/99	200.00 - 6000.00	-249.210
541	D2O2	g 6/99	200.00 - 6000.00	-144.300
542	D2S	g 6/01	200.00 - 6000.00	-24.007
543	F	g 5/97	200.00 - 20000.00	79.380
544	F+	g 3/97	298.15 - 20000.00	1766.816
545	F-	g 1/98	298.15 - 20000.00	-255.092
546	FCN	g 5/99	200.00 - 6000.00	34.328
547	FCO	g12/99	200.00 - 6000.00	-179.418
548	FO	j 9/95	200.00 - 6000.00	109.012
549	FO2,FOO	j 9/95	200.00 - 6000.00	25.400
550	FO2,OFO	j 9/95	200.00 - 6000.00	378.600
551	F2	tpis89	200.00 - 6000.00	0.000
552	F2O	g 4/99	200.00 - 6000.00	24.500
553	F2O2	j 9/95	200.00 - 6000.00	19.200
554	FS2F	j 6/76	200.00 - 6000.00	-336.435
555	Fe	g 5/97	200.00 - 20000.00	415.471
556	Fe+	g 3/98	298.15 - 20000.00	1184.218
557	Fe-	g 9/97	298.15 - 20000.00	393.338
558	Fe(CO)5	j 3/78	200.00 - 6000.00	-727.850
559	FeCL	j 6/65	200.00 - 6000.00	251.040
560	FeCL2	j12/70	200.00 - 6000.00	-141.001
561	FeCL3	j 6/65	200.00 - 6000.00	-1059.104
562	FeO	j 9/66	200.00 - 6000.00	251.040
563	Fe(OH)2	j12/66	200.00 - 6000.00	-330.536
564	Fe2CL4	j12/70	200.00 - 6000.00	-431.370
565	Fe2CL6	j 6/65	200.00 - 6000.00	-654.378
566	Ga	12/98	200.00 - 20000.00	272.000
567	Ga+	g12/98	298.15 - 20000.00	856.688
568	GaBr	tpis96	200.00 - 6000.00	-17.968
569	GaBr2	tpis96	200.00 - 6000.00	-149.181
570	GaBr3	tpis96	200.00 - 6000.00	-292.963
571	GaCL	tpis96	200.00 - 6000.00	-69.621
572	GaCL2	tpis96	200.00 - 6000.00	-220.979
573	GaCL3	tpis96	200.00 - 6000.00	-432.625
574	GaF	tpis96	200.00 - 6000.00	-232.608
575	GaF2	tpis96	200.00 - 6000.00	-516.712
576	GaF3	tpis96	200.00 - 6000.00	-921.477
577	GaH	tpis96	200.00 - 6000.00	214.323
578	GaI	tpis96	200.00 - 6000.00	44.871
579	GaI2	tpis96	200.00 - 6000.00	-28.955
580	GaI3	tpis96	200.00 - 6000.00	-115.877
581	GaO	tpis96	200.00 - 6000.00	146.824
582	GaOH	tpis96	200.00 - 6000.00	-143.630
583	Ga2Br2	tpis96	200.00 - 6000.00	-136.964

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
584	Ga2Br4	tpis96	200.00 - 6000.00	-415.820
585	Ga2Br6	tpis96	200.00 - 6000.00	-673.689
586	Ga2CL2	tpis96	200.00 - 6000.00	-220.973
587	Ga2CL4	tpis96	200.00 - 6000.00	-602.327
588	Ga2CL6	tpis96	200.00 - 6000.00	-962.464
589	Ga2F2	tpis96	200.00 - 6000.00	-606.231
590	Ga2F4	tpis96	200.00 - 6000.00	-1325.003
591	Ga2F6	tpis96	200.00 - 6000.00	-2017.624
592	Ga2I2	tpis96	200.00 - 6000.00	13.521
593	Ga2I4	tpis96	200.00 - 6000.00	-159.268
594	Ga2I6	tpis96	200.00 - 6000.00	-317.295
595	Ga2O	tpis96	200.00 - 6000.00	-99.457
596	Ge	g 3/99	200.00 - 20000.00	367.800
597	Ge+	g 3/99	298.15 - 20000.00	1134.984
598	Ge-	g 3/99	298.15 - 20000.00	245.403
599	GeBr	tpis91	200.00 - 6000.00	137.438
600	GeBr2	tpis91	200.00 - 6000.00	-60.963
601	GeBr3	tpis91	200.00 - 6000.00	-119.031
602	GeBr4	tpis91	200.00 - 6000.00	-291.000
603	GeCL	tpis91	200.00 - 6000.00	69.030
604	GeCL2	tpis91	200.00 - 6000.00	-171.000
605	GeCL3	g 6/01	200.00 - 6000.00	-266.951
606	GeCL4	tpis91	200.00 - 6000.00	-500.000
607	GeF	tpis91	200.00 - 6000.00	-70.593
608	GeF2	tpis91	200.00 - 6000.00	-574.000
609	GeF3	g 6/01	200.00 - 6000.00	-806.333
610	GeF4	tpis91	200.00 - 6000.00	-1190.150
611	GeH4	bar89	298.15 - 6000.00	90.793
612	GeI	tpis91	200.00 - 6000.00	210.969
613	GeO	tpis91	200.00 - 6000.00	-37.694
614	GeO2	tpis91	200.00 - 6000.00	-106.172
615	GeS	tpis91	200.00 - 6000.00	92.525
616	GeS2	tpis91	200.00 - 6000.00	118.818
617	Ge2	tpis91	200.00 - 6000.00	471.499
618	H	g 6/97	200.00 - 20000.00	217.999
619	H+	g10/00	298.15 - 20000.00	1536.246
620	H-	g 9/96	298.15 - 20000.00	139.031
621	HALO	tpis96	200.00 - 6000.00	1.821
622	HALO2	tpis96	200.00 - 6000.00	-355.474
623	HBO	tpis96	200.00 - 6000.00	-210.621
624	HBO+	g 1/01	298.15 - 20000.00	1175.220
625	HBO2	tpis96	200.00 - 6000.00	-560.210
626	HBS	g 2/01	200.00 - 6000.00	50.208
627	HBS+	g 1/01	298.15 - 20000.00	1129.459
628	HBr	tpis89	200.00 - 6000.00	-36.290
629	HCN	g 6/01	200.00 - 6000.00	133.082
630	HCO	g 1/01	200.00 - 6000.00	42.398
631	HCO+	g 1/01	298.15 - 20000.00	833.034
632	HCCN	tpis89	200.00 - 6000.00	610.431
633	HCCO	g 6/01	200.00 - 6000.00	176.568
634	HCL	tpis89	200.00 - 6000.00	-92.310
635	HD	tpis89	298.15 - 20000.00	0.323
636	HD+	j 9/77	298.15 - 20000.00	1496.793
637	HDO	g 5/99	200.00 - 6000.00	-245.280

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
638	HDO2	g 5/99	200.00 - 6000.00	-140.242
639	HF	tpis89	200.00 - 20000.00	-273.300
640	HI	j 9/61	200.00 - 6000.00	26.359
641	HNC	g 6/01	200.00 - 6000.00	194.378
642	HNCO	g 7/00	200.00 - 6000.00	-118.057
643	HNO	g 5/99	200.00 - 6000.00	102.033
644	HNO2	tpis89	200.00 - 6000.00	-78.452
645	HNO3	g 5/99	200.00 - 6000.00	-133.913
646	HOCL	g 1/01	200.00 - 6000.00	-75.740
647	HOF	tpis89	200.00 - 6000.00	-96.898
648	HO2	g 5/99	200.00 - 6000.00	12.552
649	HO2-	tpis89	298.15 - 6000.00	-97.630
650	HPO	tpis89	200.00 - 6000.00	-56.869
651	HSO3F	j 6/72	200.00 - 6000.00	-753.120
652	H2	tpis78	200.00 - 20000.00	0.000
653	H2+	tpis78	298.15 - 20000.00	1494.672
654	H2-	j 9/77	298.15 - 6000.00	235.168
655	HBOH	g 9/98	200.00 - 6000.00	-48.724
656	HCHO,formaldehy	g 5/01	200.00 - 6000.00	-108.580
657	HCOOH	g 6/01	200.00 - 6000.00	-378.570
658	H2F2	tpis89	200.00 - 6000.00	-569.924
659	H2O	g 8/89	200.00 - 6000.00	-241.826
660	H2O+	tpis89	298.15 - 20000.00	981.602
661	H2O2	g 6/99	200.00 - 6000.00	-135.880
662	H2S	g 4/01	200.00 - 6000.00	-20.600
663	H2SO4	tpis89	200.00 - 6000.00	-732.732
664	H2BOH	tpis96	200.00 - 6000.00	-289.634
665	HB(OH)2	tpis96	200.00 - 6000.00	-644.439
666	H3BO3	tpis96	200.00 - 6000.00	-1004.360
667	H3B3O3	tpis96	200.00 - 6000.00	-1203.761
668	H3B3O6	tpis96	200.00 - 6000.00	-2263.688
669	H3F3	tpis89	200.00 - 6000.00	-883.677
670	H3O+	tpis89	298.15 - 20000.00	598.000
671	HCOOH)2	g 6/01	200.00 - 6000.00	-820.943
672	H4F4	tpis89	200.00 - 6000.00	-1186.932
673	H5F5	tpis89	200.00 - 6000.00	-1490.188
674	H6F6	tpis89	200.00 - 6000.00	-1805.545
675	H7F7	tpis89	200.00 - 6000.00	-2099.699
676	He	g 5/97	200.00 - 20000.00	0.000
677	He+	g 3/97	298.15 - 20000.00	2378.521
678	Hg	g 1/98	200.00 - 20000.00	61.380
679	Hg+	g 7/97	298.15 - 20000.00	1074.643
680	HgBr2	g12/00	200.00 - 6000.00	-91.312
681	I	g 3/97	200.00 - 20000.00	106.760
682	I+	g10/97	298.15 - 20000.00	1121.351
683	I-	g10/97	298.15 - 20000.00	-194.596
684	IF5	tpis89	200.00 - 6000.00	-841.000
685	IF7	tpis89	200.00 - 6000.00	-961.500
686	I2	tpis89	200.00 - 6000.00	62.420
687	In	g 1/99	200.00 - 20000.00	240.700
688	In+	g 4/99	298.15 - 20000.00	6.996
689	InBr	tpis96	200.00 - 6000.00	-54.116
690	InBr2	tpis96	200.00 - 6000.00	-149.729
691	InBr3	tpis96	200.00 - 6000.00	-256.587

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
692	InCL	tpis96	200.00 - 6000.00	-72.148
693	InCL2	tpis96	200.00 - 6000.00	-201.483
694	InCL3	tpis96	200.00 - 6000.00	-369.693
695	InF	tpis96	200.00 - 6000.00	-193.420
696	InF2	tpis96	200.00 - 6000.00	-457.187
697	InF3	tpis96	200.00 - 6000.00	-863.080
698	InH	tpis96	200.00 - 6000.00	215.017
699	InI	tpis96	200.00 - 6000.00	26.417
700	InI2	tpis96	200.00 - 6000.00	-39.461
701	InI3	tpis96	200.00 - 6000.00	-105.436
702	InO	tpis96	200.00 - 6000.00	145.993
703	InOH	tpis96	200.00 - 6000.00	-124.447
704	In2Br2	tpis96	200.00 - 6000.00	-196.305
705	In2Br4	tpis96	200.00 - 6000.00	-436.509
706	In2Br6	tpis96	200.00 - 6000.00	-628.683
707	In2CL2	tpis96	200.00 - 6000.00	-232.177
708	In2CL4	tpis96	200.00 - 6000.00	-579.126
709	In2CL6	tpis96	200.00 - 6000.00	-882.340
710	In2F2	tpis96	200.00 - 6000.00	-532.234
711	In2F4	tpis96	200.00 - 6000.00	-1284.788
712	In2F6	tpis96	200.00 - 6000.00	-1960.000
713	In2I2	tpis96	200.00 - 6000.00	-27.814
714	In2I4	tpis96	200.00 - 6000.00	-199.143
715	In2I6	tpis96	200.00 - 6000.00	-319.720
716	In2O	tpis96	200.00 - 6000.00	-34.764
717	K	g 7/97	200.00 - 20000.00	89.000
718	K+	g 6/97	298.15 - 20000.00	514.008
719	K-	g 9/97	298.15 - 20000.00	34.418
720	KALF4	tpis82	200.00 - 6000.00	-1907.857
721	KBO2	tpis82	200.00 - 6000.00	-668.023
722	KCN	j 3/66	200.00 - 6000.00	79.496
723	KBr	tpis82	200.00 - 6000.00	-179.251
724	KCL	tpis82	200.00 - 6000.00	-214.575
725	KF	tpis82	200.00 - 6000.00	-328.445
726	KH	tpis82	200.00 - 6000.00	125.399
727	KI	tpis82	200.00 - 6000.00	-128.456
728	KNO2	tpis82	200.00 - 6000.00	-192.497
729	KNO3	tpis82	200.00 - 6000.00	-315.833
730	KO	tpis82	200.00 - 6000.00	64.733
731	KOH	g 9/97	200.00 - 6000.00	-232.000
732	K2	tpis82	200.00 - 6000.00	126.546
733	K2+	tpis82	298.15 - 3000.00	524.661
734	K2Br2	tpis82	200.00 - 6000.00	-538.744
735	K2CO3	tpis82	200.00 - 6000.00	-811.649
736	K2C2N2	j 3/66	200.00 - 6000.00	-8.368
737	K2CL2	tpis82	200.00 - 6000.00	-615.394
738	K2F2	tpis82	200.00 - 6000.00	-859.875
739	K2I2	tpis82	200.00 - 6000.00	-418.915
740	KLi	tpis82	200.00 - 6000.00	170.702
741	KNa	tpis82	200.00 - 6000.00	132.404
742	K2O	tpis82	200.00 - 6000.00	-74.087
743	K2O+	tpis82	298.15 - 6000.00	368.390
744	K2O2	tpis82	200.00 - 6000.00	-191.566
745	K2O2H2	g 9/97	200.00 - 6000.00	-641.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
746	K2SO4	g10/99	200.00 - 6000.00	-1095.851
747	Kr	g 8/97	200.00 - 20000.00	0.000
748	Kr+	g 7/97	298.15 - 20000.00	1356.954
749	Li	g 7/97	200.00 - 20000.00	159.300
750	Li+	g 3/97	298.15 - 20000.00	685.719
751	Li-	g 1/98	298.15 - 20000.00	93.475
752	LiALF4	tpis82	200.00 - 6000.00	-1857.288
753	LiBO2	tpis82	200.00 - 6000.00	-652.352
754	LiBr	tpis82	200.00 - 6000.00	-151.163
755	LiCL	tpis82	200.00 - 6000.00	-193.780
756	LiF	tpis89	200.00 - 6000.00	-340.945
757	LiH	tpis82	200.00 - 6000.00	139.264
758	LiI	tpis82	200.00 - 6000.00	-85.270
759	LiN	j12/66	200.00 - 6000.00	334.720
760	LiNO2	tpis82	200.00 - 6000.00	-202.031
761	LiNO3	tpis82	200.00 - 6000.00	-311.585
762	LiO	tpis82	200.00 - 6000.00	72.914
763	LiOF	j 9/65	200.00 - 6000.00	-92.048
764	LiOH	g12/96	200.00 - 6000.00	-229.000
765	LiON	j 9/66	200.00 - 6000.00	179.912
766	Li2	j12/83	200.00 - 6000.00	215.900
767	Li2+	tpis82	298.15 - 6000.00	721.611
768	Li2Br2	tpis82	200.00 - 6000.00	-495.834
769	Li2CL2	tpis82	200.00 - 6000.00	-597.539
770	Li2F2	tpis82	200.00 - 6000.00	-935.323
771	Li2I2	tpis82	200.00 - 6000.00	-362.801
772	Li2O	tpis82	200.00 - 6000.00	-167.339
773	Li2O+	tpis82	298.15 - 6000.00	439.095
774	Li2O2	tpis82	200.00 - 6000.00	-279.398
775	Li2O2H2	g12/96	200.00 - 6000.00	-737.000
776	Li2SO4	j12/78	200.00 - 6000.00	-1041.816
777	Li3+	tpis82	298.15 - 6000.00	756.591
778	Li3Br3	tpis82	200.00 - 6000.00	-824.639
779	Li3CL3	tpis82	200.00 - 6000.00	-976.107
780	Li3F3	tpis82	200.00 - 6000.00	-1524.597
781	Li3I3	tpis82	200.00 - 6000.00	-612.457
782	Mg	g 6/97	200.00 - 20000.00	147.100
783	Mg+	g 6/97	298.15 - 20000.00	891.047
784	MgBr	tpis96	200.00 - 6000.00	6.163
785	MgBr2	tpis96	200.00 - 6000.00	-306.743
786	MgCL	tpis96	200.00 - 6000.00	-54.705
787	MgCL+	g 1/01	298.15 - 20000.00	646.339
788	MgCL2	tpis96	200.00 - 6000.00	-399.170
789	MgF	tpis96	200.00 - 6000.00	-232.267
790	MgF+	g 2/01	298.15 - 20000.00	516.868
791	MgF2	tpis96	200.00 - 6000.00	-735.498
792	MgF2+	g 2/01	298.15 - 20000.00	582.692
793	MgH	tpis96	200.00 - 6000.00	229.786
794	MgI	tpis96	200.00 - 6000.00	61.206
795	MgI2	tpis96	200.00 - 6000.00	-171.706
796	MgN	j 3/64	200.00 - 6000.00	288.696
797	MgO	tpis96	200.00 - 20000.00	32.261
798	MgOH	tpis96	200.00 - 6000.00	-132.429
799	MgOH+	g 1/01	298.15 - 20000.00	615.769

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
800	Mg(OH)2	tpis96	200.00 - 6000.00	-551.996
801	MgS	tpis96	200.00 - 6000.00	120.649
802	Mg2	tpis96	200.00 - 6000.00	286.513
803	Mg2F4	j12/75	200.00 - 6000.00	-1718.369
804	Mn	g 7/97	200.00 - 20000.00	282.400
805	Mn+	g 6/97	298.15 - 20000.00	1005.871
806	Mo	g 7/97	200.00 - 20000.00	658.500
807	Mo+	g 7/97	298.15 - 20000.00	1349.013
808	Mo-	g10/97	298.15 - 20000.00	580.325
809	MoO	tpis89	200.00 - 20000.00	358.005
810	MoO2	tpis82	200.00 - 6000.00	-15.558
811	MoO3	tpis82	200.00 - 6000.00	-364.412
812	MoO3-	tpis82	298.15 - 6000.00	-655.243
813	Mo2O6	tpis82	200.00 - 6000.00	-1149.447
814	Mo3O9	tpis82	200.00 - 6000.00	-1902.031
815	Mo4O12	tpis82	200.00 - 6000.00	-2625.527
816	N	g 5/97	200.00 - 20000.00	472.680
817	N+	g 6/97	298.15 - 20000.00	1882.128
818	N-	j12/82	298.15 - 20000.00	473.538
819	NCO	g 6/01	200.00 - 6000.00	131.847
820	ND	g 4/01	200.00 - 6000.00	355.739
821	ND2	g 4/01	200.00 - 6000.00	184.837
822	ND3	g 4/01	200.00 - 6000.00	-54.752
823	NF	tpis89	200.00 - 6000.00	232.990
824	NF2	g 4/99	200.00 - 6000.00	34.421
825	NF3	g 4/99	200.00 - 6000.00	-131.700
826	NH	g 4/99	200.00 - 20000.00	357.032
827	NH+	g 5/99	298.15 - 20000.00	1665.788
828	NHF	tpis89	200.00 - 6000.00	112.000
829	NHF2	tpis89	200.00 - 6000.00	-103.000
830	NH2	g 3/01	200.00 - 6000.00	189.135
831	NH2F	tpis89	200.00 - 6000.00	-75.000
832	NH3	tpis89	200.00 - 6000.00	-45.940
833	NH2OH	tpis89	200.00 - 6000.00	-50.000
834	NH4+	tpis89	298.15 - 6000.00	644.905
835	NO	tpis89	200.00 - 20000.00	91.271
836	NO+	tpis89	298.15 - 20000.00	990.810
837	NOCL	g 4/99	200.00 - 6000.00	52.699
838	NOF	g 4/99	200.00 - 6000.00	-65.000
839	NOF3	tpis89	200.00 - 6000.00	-187.000
840	NO2	g 4/99	200.00 - 6000.00	34.193
841	NO2-	tpis89	298.15 - 6000.00	-200.036
842	NO2CL	g 4/99	200.00 - 6000.00	12.500
843	NO2F	g 4/99	200.00 - 6000.00	-109.000
844	NO3	j12/64	200.00 - 6000.00	71.128
845	NO3-	tpis89	298.15 - 6000.00	-310.780
846	NO3F	tpis89	200.00 - 6000.00	15.000
847	N2	tpis78	200.00 - 20000.00	0.000
848	N2+	tpis89	298.15 - 20000.00	1509.508
849	N2-	j 9/77	298.15 - 20000.00	148.183
850	NCN	g 6/01	200.00 - 6000.00	500.457
851	N2D2,ci	s 6/01	200.00 - 6000.00	202.857
852	N2F2	tpis89	200.00 - 6000.00	62.374
853	N2F4	tpis89	200.00 - 6000.00	-22.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
854	N2H2	g 5/99	200.00 - 6000.00	211.859
855	NH2NO2	tpis89	200.00 - 6000.00	-26.000
856	N2H4	g 4/99	200.00 - 6000.00	95.180
857	N2O	g 4/99	200.00 - 6000.00	81.600
858	N2O+	j12/70	298.15 - 6000.00	1332.957
859	N2O3	g 4/99	200.00 - 6000.00	86.631
860	N2O4	tpis89	200.00 - 6000.00	11.111
861	N2O5	g 4/99	200.00 - 6000.00	13.300
862	N3	tpis89	200.00 - 6000.00	436.000
863	N3H	g 4/99	200.00 - 6000.00	294.000
864	Na	g 8/97	200.00 - 20000.00	107.500
865	Na+	g 1/98	298.15 - 20000.00	609.543
866	Na-	g 4/97	298.15 - 20000.00	48.453
867	NaALF4	tpis82	200.00 - 6000.00	-1857.842
868	NaBO2	tpis82	200.00 - 6000.00	-633.449
869	NaBr	tpis82	200.00 - 6000.00	-145.929
870	NaCN	j 3/66	200.00 - 6000.00	94.266
871	NaCL	tpis82	200.00 - 6000.00	-181.545
872	NaF	tpis82	200.00 - 6000.00	-295.157
873	NaH	tpis82	200.00 - 6000.00	140.835
874	NaI	tpis82	200.00 - 6000.00	-90.638
875	NaLi	tpis82	200.00 - 6000.00	178.598
876	NaNO2	g10/99	200.00 - 6000.00	-166.293
877	NaNO3	tpis82	200.00 - 6000.00	-285.529
878	NaO	tpis82	200.00 - 6000.00	106.505
879	NaOH	g12/96	200.00 - 6000.00	-191.000
880	NaOH+	g 2/01	298.15 - 20000.00	683.862
881	Na2	tpis82	200.00 - 6000.00	142.339
882	Na2Br2	tpis82	200.00 - 6000.00	-480.848
883	Na2CL2	tpis82	200.00 - 6000.00	-564.402
884	Na2F2	tpis82	200.00 - 6000.00	-834.063
885	Na2I2	tpis82	200.00 - 6000.00	-356.870
886	Na2O	tpis82	200.00 - 6000.00	-16.560
887	Na2O+	tpis82	298.15 - 6000.00	520.834
888	Na2O2	tpis82	200.00 - 6000.00	-123.930
889	Na2O2H2	g 8/01	200.00 - 6000.00	-624.000
890	Na2SO4	tpis82	200.00 - 6000.00	-1040.132
891	Na3CL3	tpis82	200.00 - 6000.00	-912.675
892	Na3F3	tpis82	200.00 - 6000.00	-1348.015
893	Nb	g 3/98	200.00 - 20000.00	723.113
894	Nb+	g 7/97	298.15 - 20000.00	1393.605
895	Nb-	g 9/97	298.15 - 20000.00	631.054
896	NbCL5	j12/74	200.00 - 6000.00	-703.330
897	NbO	tpis82	200.00 - 20000.00	210.989
898	NbOCL3	bar 89	298.15 - 6000.00	-752.300
899	NbO2	tpis82	200.00 - 6000.00	-201.267
900	Ne	g 5/97	200.00 - 20000.00	0.000
901	Ne+	g 3/97	298.15 - 20000.00	2086.966
902	Ni	g 8/97	200.00 - 20000.00	430.117
903	Ni+	g 8/97	298.15 - 20000.00	1172.595
904	Ni-	g 9/97	298.15 - 20000.00	311.764
905	NiCL	j 9/77	200.00 - 6000.00	182.004
906	NiCL2	j 9/77	200.00 - 6000.00	-73.931
907	NiO	g12/00	200.00 - 6000.00	297.064

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
908	NiS	j12/76	200.00 - 6000.00	357.419
909	O	g 5/97	200.00 - 20000.00	249.175
910	O+	g 8/97	298.15 - 20000.00	1568.787
911	O-	g 1/97	298.15 - 20000.00	101.846
912	OD	tpis89	200.00 - 6000.00	37.222
913	OD-	tpis89	298.15 - 6000.00	-145.383
914	OH	tpis78	200.00 - 20000.00	39.344
915	OH+	g 6/99	298.15 - 20000.00	1290.332
916	OH-	tpis89	298.15 - 6000.00	-143.190
917	O2	tpis89	200.00 - 20000.00	0.000
918	O2+	tpis89	298.15 - 20000.00	1171.828
919	O2-	g11/99	298.15 - 6000.00	-48.028
920	O3	tpis89	200.00 - 6000.00	141.800
921	P	g 5/97	200.00 - 20000.00	316.500
922	P+	g 4/97	298.15 - 20000.00	1336.453
923	P-	g 4/97	298.15 - 20000.00	238.827
924	PCL	tpis89	200.00 - 6000.00	134.615
925	PCL2	tpis89	200.00 - 6000.00	-54.292
926	PCL2-	tpis89	298.15 - 6000.00	-356.285
927	PCL3	tpis89	200.00 - 6000.00	-289.500
928	PCL5	tpis89	200.00 - 6000.00	-376.000
929	PF	tpis89	200.00 - 6000.00	-47.945
930	PF+	j 6/77	298.15 - 20000.00	901.518
931	PF-	j 6/77	298.15 - 20000.00	-164.046
932	PFCL	tpis89	200.00 - 6000.00	-283.184
933	PFCL-	tpis89	298.15 - 6000.00	-529.269
934	PFCL2	tpis89	200.00 - 6000.00	-511.925
935	PFCL4	tpis89	200.00 - 6000.00	-635.016
936	PF2	tpis89	200.00 - 6000.00	-513.104
937	PF2-	tpis89	298.15 - 6000.00	-709.338
938	PF2CL	tpis89	200.00 - 6000.00	-735.077
939	PF2CL3	tpis89	200.00 - 6000.00	-878.745
940	PF3	tpis89	200.00 - 6000.00	-957.400
941	PF3CL2	tpis89	200.00 - 6000.00	-1122.023
942	PF4CL	tpis89	200.00 - 6000.00	-1364.909
943	PF5	tpis89	200.00 - 6000.00	-1593.300
944	PH	tpis89	200.00 - 6000.00	230.752
945	PH2	tpis89	200.00 - 6000.00	119.553
946	PH2-	tpis89	298.15 - 6000.00	-9.265
947	PH3	j 6/62	200.00 - 6000.00	5.439
948	PN	tpis89	200.00 - 6000.00	171.487
949	PO	tpis89	200.00 - 6000.00	-27.858
950	PO-	tpis89	298.15 - 6000.00	-140.067
951	POCL3	tpis89	200.00 - 6000.00	-568.400
952	POFCL2	tpis89	200.00 - 6000.00	-793.889
953	POF2CL	tpis89	200.00 - 6000.00	-1022.607
954	POF3	tpis89	200.00 - 6000.00	-1252.000
955	PO2	tpis89	200.00 - 6000.00	-281.527
956	PO2-	tpis89	298.15 - 6000.00	-597.624
957	PS	tpis89	200.00 - 6000.00	150.431
958	P2	tpis89	200.00 - 6000.00	144.000
959	P2O3	tpis89	200.00 - 6000.00	-684.645
960	P2O4	tpis89	200.00 - 6000.00	-933.755
961	P2O5	tpis89	200.00 - 6000.00	-1124.370

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
962	P3	tpis89	200.00 - 6000.00	210.000
963	P3O6	tpis89	200.00 - 6000.00	-1575.681
964	P4	tpis89	200.00 - 6000.00	58.900
965	P4O6	tpis89	200.00 - 6000.00	-1606.000
966	P4O7	tpis89	200.00 - 6000.00	-1984.448
967	P4O8	tpis89	200.00 - 6000.00	-2302.214
968	P4O9	tpis89	200.00 - 6000.00	-2613.979
969	P4O10	tpis89	200.00 - 6000.00	-2906.223
970	Pb	g 8/97	200.00 - 20000.00	195.200
971	Pb+	g10/97	298.15 - 20000.00	916.997
972	Pb-	g 9/97	298.15 - 20000.00	153.882
973	PbBr	tpis91	200.00 - 6000.00	64.821
974	PbBr2	tpis91	200.00 - 6000.00	-103.908
975	PbBr3	tpis91	200.00 - 6000.00	-104.011
976	PbBr4	tpis91	200.00 - 6000.00	-182.436
977	PbCL	tpis91	200.00 - 6000.00	8.819
978	PbCL2	tpis91	200.00 - 6000.00	-175.547
979	PbCL3	tpis91	200.00 - 6000.00	-177.654
980	PbCL4	tpis91	200.00 - 6000.00	-327.430
981	PbF	tpis91	200.00 - 6000.00	-98.868
982	PbF	g 5/99	200.00 - 6000.00	-98.867
983	PbF2	tpis91	200.00 - 6000.00	-443.427
984	PbF3	tpis91	200.00 - 6000.00	-489.573
985	PbF4	tpis91	200.00 - 6000.00	-799.925
986	PbI	tpis91	200.00 - 6000.00	108.904
987	PbI2	tpis91	200.00 - 6000.00	-10.253
988	PbI3	tpis91	200.00 - 6000.00	21.755
989	PbI4	tpis91	200.00 - 6000.00	-41.226
990	PbO	tpis91	200.00 - 6000.00	68.137
991	PbO2	tpis91	200.00 - 6000.00	136.153
992	PbS	tpis91	200.00 - 6000.00	127.945
993	PbS2	tpis91	200.00 - 6000.00	244.049
994	Pb2	g 5/99	200.00 - 6000.00	305.561
995	Rb	g 1/98	200.00 - 20000.00	80.900
996	Rb+	g 1/98	298.15 - 20000.00	490.129
997	Rb-	g 9/97	298.15 - 20000.00	27.819
998	RbBO2	tpis82	200.00 - 6000.00	-678.977
999	RbBr	tpis82	200.00 - 6000.00	-191.511
1000	RbCL	tpis82	200.00 - 6000.00	-223.323
1001	RbF	tpis82	200.00 - 6000.00	-333.512
1002	RbH	tpis82	200.00 - 6000.00	119.324
1003	RbI	tpis82	200.00 - 6000.00	-138.481
1004	RbK	tpis82	200.00 - 6000.00	120.013
1005	RbLi	tpis82	200.00 - 6000.00	164.181
1006	RbNO2	tpis82	200.00 - 6000.00	-187.630
1007	RbNO3	tpis82	200.00 - 6000.00	-314.972
1008	RbNa	tpis82	200.00 - 6000.00	131.470
1009	RbO	tpis82	200.00 - 6000.00	52.489
1010	RbOH	g 9/97	200.00 - 6000.00	-238.000
1011	Rb2Br2	tpis82	200.00 - 6000.00	-551.801
1012	Rb2CL2	tpis82	200.00 - 6000.00	-618.374
1013	Rb2F2	tpis82	200.00 - 6000.00	-854.913
1014	Rb2I2	tpis82	200.00 - 6000.00	-432.956
1015	Rb2O	tpis82	200.00 - 6000.00	-108.929

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1016	Rb2O2	tpis82	200.00 - 6000.00	-215.848
1017	Rb2O2H2	g 9/97	200.00 - 6000.00	-639.000
1018	Rb2SO4	g10/99	200.00 - 6000.00	-1096.592
1019	Rn	g 5/97	200.00 - 20000.00	0.000
1020	Rn+	g 1/97	298.15 - 20000.00	1043.270
1021	S	g 5/97	200.00 - 20000.00	277.170
1022	S+	g 1/98	298.15 - 20000.00	1282.496
1023	S-	g 4/97	298.15 - 20000.00	70.369
1024	SCL	j 6/78	200.00 - 6000.00	156.465
1025	SCL2	j 6/78	200.00 - 6000.00	-17.573
1026	SCL2+	j 6/78	298.15 - 20000.00	901.383
1027	SD	j 6/77	200.00 - 6000.00	138.491
1028	SF	tpis89	200.00 - 6000.00	15.446
1029	SF+	g 1/01	298.15 - 20000.00	994.570
1030	SF-	tpis89	298.15 - 6000.00	-231.347
1031	SF2	tpis89	200.00 - 6000.00	-293.189
1032	SF2+	g 1/01	298.15 - 20000.00	706.016
1033	SF2-	g 1/01	298.15 - 20000.00	-394.795
1034	SF3	tpis89	200.00 - 6000.00	-504.101
1035	SF3+	j12/76	298.15 - 20000.00	393.583
1036	SF3-	tpis89	298.15 - 6000.00	-790.124
1037	SF4	tpis89	200.00 - 6000.00	-760.000
1038	SF4+	j12/76	298.15 - 20000.00	416.112
1039	SF4-	j12/76	298.15 - 20000.00	-887.464
1040	SF5	tpis89	200.00 - 6000.00	-902.663
1041	SF5+	j12/77	298.15 - 20000.00	172.644
1042	SF5-	tpis89	298.15 - 6000.00	-1204.622
1043	SF6	tpis89	200.00 - 6000.00	-1219.400
1044	SF6-	j 6/77	298.15 - 20000.00	-1341.876
1045	SH	tpis89	200.00 - 6000.00	140.412
1046	SH-	tpis89	298.15 - 6000.00	-88.297
1047	SN	tpis89	200.00 - 6000.00	267.388
1048	SO	tpis89	200.00 - 6000.00	4.760
1049	SO-	tpis89	298.15 - 6000.00	-105.968
1050	SOF2	tpis89	200.00 - 6000.00	-584.952
1051	SO2	tpis89	200.00 - 6000.00	-296.810
1052	SO2-	tpis89	298.15 - 6000.00	-408.606
1053	SO2CL2	j 6/71	200.00 - 6000.00	-354.803
1054	SO2FCL	j 6/71	200.00 - 6000.00	-556.472
1055	SO2F2	tpis89	200.00 - 6000.00	-760.000
1056	SO3	tpis89	200.00 - 6000.00	-395.900
1057	S2	tpis89	200.00 - 6000.00	128.600
1058	S2-	tpis89	298.15 - 6000.00	-37.132
1059	S2CL2	g12/00	200.00 - 6000.00	-16.736
1060	S2F2	j 6/76	200.00 - 6000.00	-401.413
1061	S2O	tpis89	200.00 - 6000.00	-56.035
1062	S3	tpis89	200.00 - 6000.00	144.738
1063	S4	tpis89	200.00 - 6000.00	135.632
1064	S5	tpis89	200.00 - 6000.00	132.993
1065	S6	tpis89	200.00 - 6000.00	101.315
1066	S7	tpis89	200.00 - 6000.00	111.890
1067	S8	tpis89	200.00 - 6000.00	101.277
1068	Sc	g 1/99	200.00 - 20000.00	377.700
1069	Sc+	g 7/97	298.15 - 20000.00	1017.145

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1070	Sc-	g 9/97	298.15 - 20000.00	352.559
1071	ScO	tpis89	200.00 - 20000.00	-55.065
1072	ScO+	g10/99	298.15 - 20000.00	561.210
1073	ScO2	tpis82	200.00 - 6000.00	-413.651
1074	Sc2O	tpis82	200.00 - 6000.00	-23.044
1075	Sc2O2	tpis82	200.00 - 6000.00	-490.571
1076	Si	g 8/97	200.00 - 20000.00	450.000
1077	Si+	g 4/97	298.15 - 20000.00	1242.508
1078	Si-	g 4/97	298.15 - 20000.00	308.818
1079	SiBr	tpis91	200.00 - 6000.00	175.157
1080	SiBr2	tpis91	200.00 - 6000.00	-51.000
1081	SiBr3	tpis91	200.00 - 6000.00	-157.000
1082	SiBr4	tpis91	200.00 - 6000.00	-415.800
1083	SiC	tpis91	200.00 - 6000.00	734.946
1084	SiC2	tpis91	200.00 - 6000.00	631.361
1085	SiCL	tpis91	200.00 - 6000.00	142.363
1086	SiCL2	tpis91	200.00 - 6000.00	-163.069
1087	SiCL3	tpis91	200.00 - 6000.00	-336.272
1088	SiCL4	tpis91	200.00 - 6000.00	-662.200
1089	SiF	tpis91	200.00 - 6000.00	-25.233
1090	SiFCL	tpis91	200.00 - 6000.00	-377.827
1091	SiF2	tpis91	200.00 - 6000.00	-592.838
1092	SiF3	tpis91	200.00 - 6000.00	-996.437
1093	SiF4	g 6/01	200.00 - 6000.00	-1615.780
1094	SiH	tpis91	200.00 - 6000.00	368.636
1095	SiH+	j12/71	298.15 - 6000.00	1147.671
1096	SiHBr3	j12/76	200.00 - 6000.00	-302.922
1097	SiHCL	tpis91	200.00 - 6000.00	54.946
1098	SiHCL3	j12/76	200.00 - 6000.00	-496.222
1099	SiHF	tpis91	200.00 - 6000.00	-162.657
1100	SiHF3	j 6/76	200.00 - 6000.00	-1200.808
1101	SiHI3	j12/76	200.00 - 6000.00	-74.475
1102	SiH2	g 3/01	200.00 - 6000.00	273.333
1103	SiH2Br2	j12/76	200.00 - 6000.00	-190.372
1104	SiH2CL2	j12/76	200.00 - 6000.00	-320.494
1105	SiH2F2	j 6/76	200.00 - 6000.00	-790.776
1106	SiH2I2	j12/76	200.00 - 6000.00	-38.074
1107	SiH3	g 3/99	200.00 - 6000.00	204.357
1108	SiH3Br	j12/76	200.00 - 6000.00	-78.241
1109	SiH3CL	j12/76	200.00 - 6000.00	-141.838
1110	SiH3F	j 6/76	200.00 - 6000.00	-376.560
1111	SiH3I	j12/76	200.00 - 6000.00	-2.092
1112	SiH4	tpis91	200.00 - 6000.00	34.700
1113	SiI	tpis91	200.00 - 6000.00	262.953
1114	SiI2	j12/76	200.00 - 6000.00	92.466
1115	SiN	g 5/99	200.00 - 6000.00	403.668
1116	SiO	tpis91	200.00 - 6000.00	-98.842
1117	SiO2	tpis91	200.00 - 6000.00	-322.073
1118	SiS	tpis91	200.00 - 6000.00	108.194
1119	SiS2	tpis91	200.00 - 6000.00	7.023
1120	Si2	tpis91	200.00 - 6000.00	580.196
1121	Si2C	tpis91	200.00 - 6000.00	554.094
1122	Si2F6	g 6/01	200.00 - 6000.00	-2383.290
1123	Si2N	j 3/67	200.00 - 6000.00	397.480

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1124	Si3	g 7/95	200.00 - 6000.00	627.867
1125	Sn	g 7/97	200.00 - 20000.00	301.200
1126	Sn+	g 7/97	298.15 - 20000.00	1015.950
1127	Sn-	g 9/97	298.15 - 20000.00	179.496
1128	SnBr	tpis91	200.00 - 6000.00	75.644
1129	SnBr2	tpis91	200.00 - 6000.00	-118.975
1130	SnBr3	tpis91	200.00 - 6000.00	-158.716
1131	SnBr4	tpis91	200.00 - 6000.00	-324.217
1132	SnCL	tpis91	200.00 - 6000.00	34.659
1133	SnCL2	tpis91	200.00 - 6000.00	-202.648
1134	SnCL3	tpis91	200.00 - 6000.00	-292.372
1135	SnCL4	tpis91	200.00 - 6000.00	-478.466
1136	SnF	tpis91	200.00 - 6000.00	-95.017
1137	SnF2	tpis91	200.00 - 6000.00	-510.957
1138	SnF3	tpis91	200.00 - 6000.00	-646.630
1139	SnF4	tpis91	200.00 - 6000.00	-1024.767
1140	SnI	tpis91	200.00 - 6000.00	172.725
1141	SnI2	tpis91	200.00 - 6000.00	-8.067
1142	SnI3	tpis91	200.00 - 6000.00	-8.018
1143	SnI4	tpis91	200.00 - 6000.00	-118.854
1144	SnO	tpis91	200.00 - 6000.00	21.911
1145	SnO2	tpis91	200.00 - 6000.00	11.680
1146	SnS	tpis91	200.00 - 6000.00	111.099
1147	SnS2	tpis91	200.00 - 6000.00	149.646
1148	Sn2	tpis91	200.00 - 6000.00	421.344
1149	Sr	g 1/98	200.00 - 20000.00	160.500
1150	Sr+	g 1/98	298.15 - 20000.00	716.166
1151	SrBr	tpis96	200.00 - 20000.00	-63.918
1152	SrBr2	tpis96	200.00 - 6000.00	-406.726
1153	SrCL	tpis96	200.00 - 20000.00	-127.868
1154	SrCL+	g 8/98	298.15 - 20000.00	408.112
1155	SrCL2	tpis96	200.00 - 6000.00	-484.814
1156	SrF	tpis96	200.00 - 20000.00	-303.553
1157	SrF+	g 8/98	298.15 - 20000.00	209.468
1158	SrF2	tpis96	200.00 - 6000.00	-784.794
1159	SrH	tpis96	200.00 - 6000.00	219.227
1160	SrI	tpis96	200.00 - 20000.00	-7.852
1161	SrI2	tpis96	200.00 - 6000.00	-278.219
1162	SrO	tpis96	200.00 - 20000.00	-14.208
1163	SrO+	g 8/98	298.15 - 20000.00	630.054
1164	SrOH	tpis96	200.00 - 6000.00	-194.086
1165	SrOH+	tpis96	298.15 - 6000.00	310.170
1166	Sr(OH)2	tpis96	200.00 - 6000.00	-596.695
1167	SrS	tpis96	200.00 - 6000.00	104.351
1168	Sr2	tpis96	200.00 - 6000.00	307.570
1169	Ta	g 7/97	200.00 - 20000.00	782.519
1170	Ta+	g 7/97	298.15 - 20000.00	1549.679
1171	Ta-	g 9/97	298.15 - 20000.00	745.469
1172	TaCL5	j12/74	200.00 - 6000.00	-764.835
1173	TaO	tpis89	200.00 - 20000.00	242.535
1174	TaO2	tpis82	200.00 - 6000.00	-173.662
1175	Ti	g 7/97	200.00 - 20000.00	473.000
1176	Ti+	g 7/97	298.15 - 20000.00	1137.624
1177	Ti-	g 9/97	298.15 - 20000.00	459.204

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1178	TiCL	j12/68	200.00 - 6000.00	150.851
1179	TiCL2	j12/68	200.00 - 6000.00	-237.230
1180	TiCL3	j12/68	200.00 - 6000.00	-539.320
1181	TiCL4	j12/67	200.00 - 6000.00	-763.160
1182	TiO	tpis89	200.00 - 20000.00	49.504
1183	TiO+	tpis82	298.15 - 20000.00	685.321
1184	TiOCL	j 9/63	200.00 - 6000.00	-244.262
1185	TiOCL2	j 9/63	200.00 - 6000.00	-545.552
1186	TiO2	g10/99	200.00 - 6000.00	-305.430
1187	U	g 7/00	200.00 - 20000.00	535.000
1188	UF	tpis82	200.00 - 20000.00	-49.251
1189	UF+	tpis82	298.15 - 20000.00	557.059
1190	UF-	g12/99	298.15 - 20000.00	-155.679
1191	UF2	tpis82	200.00 - 20000.00	-535.037
1192	UF2+	tpis82	298.15 - 20000.00	70.446
1193	UF2-	tpis82	298.15 - 20000.00	-678.233
1194	UF3	tpis82	200.00 - 20000.00	-1060.959
1195	UF3+	tpis82	298.15 - 20000.00	-284.745
1196	UF3-	tpis82	298.15 - 20000.00	-1186.441
1197	UF4	tpis82	200.00 - 20000.00	-1606.157
1198	UF4+	tpis82	298.15 - 20000.00	-641.539
1199	UF4-	tpis82	298.15 - 20000.00	-1728.335
1200	UF5	tpis82	200.00 - 20000.00	-1949.824
1201	UF5+	tpis82	298.15 - 20000.00	-853.617
1202	UF5-	tpis82	298.15 - 20000.00	-2289.431
1203	UF6	tpis82	200.00 - 20000.00	-2148.642
1204	UF6-	tpis82	298.15 - 20000.00	-2691.306
1205	UO	tpis82	200.00 - 20000.00	30.489
1206	UO+	tpis82	298.15 - 20000.00	580.972
1207	UOF	tpis82	200.00 - 6000.00	-542.183
1208	UOF2	tpis82	200.00 - 6000.00	-1115.510
1209	UOF3	tpis82	200.00 - 6000.00	-1510.638
1210	UOF4	tpis82	200.00 - 6000.00	-1785.612
1211	UO2	tpis82	200.00 - 20000.00	-477.820
1212	UO2+	tpis82	298.15 - 20000.00	51.494
1213	UO2-	tpis82	298.15 - 20000.00	-573.700
1214	UO2F	tpis82	200.00 - 6000.00	-997.935
1215	UO2F2	tpis82	200.00 - 6000.00	-1354.232
1216	UO3	tpis82	200.00 - 20000.00	-799.239
1217	UO3-	tpis82	298.15 - 20000.00	-1305.155
1218	V	g 7/97	200.00 - 20000.00	517.267
1219	V+	g 7/97	298.15 - 20000.00	1173.745
1220	V-	g 9/97	298.15 - 20000.00	460.386
1221	VCL4	g10/00	200.00 - 6000.00	-527.058
1222	VN	j12/73	200.00 - 6000.00	523.000
1223	VO	tpis89	200.00 - 20000.00	148.583
1224	VO2	tpis82	200.00 - 6000.00	-232.698
1225	V4O10	g10/99	200.00 - 6000.00	-2825.164
1226	W	g 4/98	200.00 - 20000.00	851.244
1227	W+	g 7/97	298.15 - 20000.00	1627.841
1228	W-	g 1/99	298.15 - 20000.00	766.392
1229	WCL6	j12/66	200.00 - 6000.00	-493.712
1230	WO	tpis82	200.00 - 20000.00	401.736
1231	WOCL4	j 6/67	200.00 - 6000.00	-573.493

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o$(298.15)
1232	WO2	tpis82	200.00 - 6000.00	29.062
1233	WO2CL2	j 6/73	200.00 - 6000.00	-671.532
1234	WO3	tpis82	200.00 - 6000.00	-319.725
1235	WO3-	tpis82	298.15 - 6000.00	-650.476
1236	(WO3)2	tpis82	200.00 - 6000.00	-1210.443
1237	(WO3)3	tpis82	200.00 - 6000.00	-2013.291
1238	(WO3)4	tpis82	200.00 - 6000.00	-2817.434
1239	(WO3)5	tpis82	200.00 - 6000.00	-3551.492
1240	Xe	g 1/99	200.00 - 20000.00	0.000
1241	Xe+	g 3/97	298.15 - 20000.00	1176.552
1242	Zn	g 6/97	200.00 - 20000.00	130.400
1243	Zn+	g 6/97	298.15 - 20000.00	1043.000
1244	Zr	g 1/98	200.00 - 20000.00	599.319
1245	Zr+	g 1/98	298.15 - 20000.00	1246.246
1246	Zr-	g 2/98	298.15 - 20000.00	552.952
1247	ZrN	j 6/63	200.00 - 6000.00	713.372
1248	ZrO	tpis82	200.00 - 20000.00	83.923
1249	ZrO+	tpis82	298.15 - 20000.00	720.614
1250	ZrO2	g10/99	200.00 - 6000.00	-317.043
1251	Ag(cr)	coda89	200.00 - 1235.08	0.000
1252	Ag(L)	coda89	1235.08 - 6000.00	0.000
1253	AL(cr)	coda89	200.00 - 933.61	0.000
1254	AL(L)	coda89	933.61 - 6000.00	0.000
1255	ALBr3(cr	tpis96	200.00 - 371.16	-511.500
1256	ALBr3(L)	tpis96	371.16 - 6000.00	-511.500
1257	ALCL3(cr)	tpis96	200.00 - 465.70	-705.100
1258	ALCL3(L)	tpis96	465.70 - 6000.00	-705.100
1259	ALF3(II)	tpis96	100.00 - 728.00	-1510.400
1260	ALF3(I)	tpis96	728.00 - 2100.00	-1510.400
1261	ALH3(a)	tpis96	200.00 - 500.00	-11.400
1262	ALI3(cr)	tpis96	298.15 - 461.47	-302.900
1263	ALI3(L)	tpis96	461.47 - 6000.00	-302.900
1264	ALN(cr)	tpis96	100.00 - 1800.00	-319.000
1265	ALN(L)	tpis96	1800.00 - 6000.00	-319.000
1266	AL(OH)3(a)	tpis96	100.00 - 500.00	-1293.500
1267	AL2O3(a)	tpis96	200.00 - 2327.00	-1675.700
1268	AL2O3(L)	tpis96	2327.00 - 6000.00	-1675.700
1269	AL2S3(a)	tpis96	100.00 - 1273.00	-648.500
1270	AL2S3(b)	tpis96	1273.00 - 1373.00	-648.500
1271	AL2S3(L)	tpis96	1373.00 - 6000.00	-648.500
1272	AL2SiO5(an)	j 9/67	200.00 - 3000.00	-2592.072
1273	AL4C3(cr)	tpis96	100.00 - 2500.00	-206.900
1274	B(b)	j 6/83	200.00 - 2350.00	0.000
1275	B(L)	j 6/83	2350.00 - 6000.00	0.000
1276	BN(cr)	tpis96	200.00 - 3240.00	-251.000
1277	BN(L)	tpis96	3240.00 - 6000.00	-251.000
1278	B2O3(cr)	tpis96	100.00 - 723.00	-1273.500
1279	B2O3(L)	tpis96	723.00 - 6000.00	-1273.500
1280	B2S3(cr)	tpis96	298.15 - 840.00	-243.000
1281	B2S3(L)	tpis96	840.00 - 6000.00	-243.000
1282	B3O3H3(cr)	j 3/65	298.15 - 2000.00	-1262.313
1283	B4C(cr)	tpis96	200.00 - 2743.00	-62.000
1284	B4C(L)	j 6/83	2743.00 - 6000.00	-62.000
1285	Ba(cr)	srd 93	80.00 - 1000.00	0.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1286	Ba(L)	srd 93	1000.00 - 6000.00	0.000
1287	BaBr2(cr)	tpis96	298.00 - 1130.00	-752.000
1288	BaBr2(L)	tpis96	1130.00 - 6000.00	-752.000
1289	BaCO3(a)	tpis96	200.00 - 1083.00	-1214.000
1290	BaCO3(b)	tpis96	1083.00 - 1233.00	-1214.000
1291	BaCO3(c)	tpis96	1233.00 - 1828.00	-1214.000
1292	BaCO3(L)	tpis96	1828.00 - 6000.00	-1214.000
1293	BaCL2(a)	tpis96	100.00 - 1198.00	-855.200
1294	BaCL2(b)	tpis96	1198.00 - 1234.00	-855.200
1295	BaCL2(L)	tpis96	1234.00 - 6000.00	-855.200
1296	BaF2(a)	tpis96	100.00 - 1240.00	-1206.000
1297	BaF2(b)	tpis96	1240.00 - 1480.00	-1206.000
1298	BaF2(c)	tpis96	1480.00 - 1641.00	-1206.000
1299	BaF2(L)	tpis96	1641.00 - 6000.00	-1206.000
1300	BaI2(cr)	tpis96	100.00 - 984.00	-606.000
1301	BaI2(L)	tpis96	984.00 - 6000.00	-606.000
1302	BaH2(a)	tpis96	298.15 - 871.00	-190.000
1303	BaH2(b)	tpis96	871.00 - 1473.00	-190.000
1304	BaH2(L)	tpis96	1473.00 - 6000.00	-190.000
1305	BaO(cr)	tpis96	200.00 - 2246.00	-548.000
1306	BaO(L)	tpis96	2246.00 - 6000.00	-548.000
1307	Ba(OH)2(b)	tpis96	100.00 - 519.00	-940.600
1308	Ba(OH)2(a)	tpis96	519.00 - 681.00	-940.600
1309	Ba(OH)2(L)	tpis96	681.00 - 6000.00	-940.600
1310	BaS(cr)	tpis96	200.00 - 2500.00	-470.000
1311	BaS(L)	tpis96	2500.00 - 6000.00	-470.000
1312	BaSO4(a)	tpis96	200.00 - 1423.00	-1470.000
1313	BaSO4(b)	tpis96	1423.00 - 1853.00	-1470.000
1314	BaSO4(L)	tpis96	1853.00 - 6000.00	-1470.000
1315	Be(a)	srd 93	100.00 - 1543.00	0.000
1316	Be(b)	srd 93	1543.00 - 1563.00	0.000
1317	Be(L)	srd 93	1563.00 - 6000.00	0.000
1318	BeAL2O4(cr)	j12/79	200.00 - 2146.00	-2300.782
1319	BeAL2O4(L)	j12/79	2146.00 - 6000.00	-2300.782
1320	BeBr2(cr)	tpis96	298.15 - 781.00	-358.000
1321	BeBr2(L)	tpis96	781.00 - 6000.00	-358.000
1322	BeCO3(cr)	tpis96	298.00 - 6000.00	-1045.000
1323	BeCL2(a)	tpis96	200.00 - 676.00	-496.200
1324	BeCL2(b)	tpis96	676.00 - 688.00	-496.200
1325	BeCL2(L)	tpis96	688.00 - 6000.00	-496.200
1326	BeF2(a)	tpis96	200.00 - 493.00	-1027.000
1327	BeF2(b)	tpis96	493.00 - 823.00	-1027.000
1328	BeF2(L)	tpis96	823.00 - 6000.00	-1027.000
1329	BeI2(cr)	tpis96	298.15 - 763.00	-191.000
1330	BeI2(L)	tpis96	763.00 - 6000.00	-191.000
1331	BeO(a)	tpis96	200.00 - 2373.00	-609.400
1332	BeO(b)	tpis96	2373.00 - 2851.00	-609.400
1333	BeO(L)	tpis96	2851.00 - 6000.00	-609.400
1334	Be(OH)2(b)	tpis96	200.00 - 6000.00	-905.700
1335	BeS(cr)	tpis96	298.00 - 6000.00	-236.000
1336	BeSO4(a)	tpis96	200.00 - 861.00	-1200.000
1337	BeSO4(b)	tpis96	861.00 - 912.00	-1200.000
1338	BeSO4(c)	tpis96	912.00 - 1400.00	-1200.000
1339	BeSO4(L)	tpis96	1400.00 - 6000.00	-1200.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range			$\Delta_f H^\circ$(298.15)
1340	Be2C(s)	bar 89	298.15	-	2400.00	-116.985
1341	Be2C(L)	bar 89	2400.00	-	6000.00	-116.985
1342	Be3N2(a)	tpis96	200.00	-	1673.00	-588.000
1343	Be3N2(b)	tpis96	1673.00	-	2473.00	-588.000
1344	Be3N2(L)	tpis96	2473.00	-	6000.00	-588.000
1345	Br2(cr)	tpis89	200.00	-	265.90	0.000
1346	Br2(L)	tpis89	265.90	-	6000.00	0.000
1347	C(gr)	n 4/83	200.00	-	6000.00	0.000
1348	Ca(a)	srd 93	200.00	-	716.00	0.000
1349	Ca(b)	srd 93	716.00	-	1115.00	0.000
1350	Ca(L)	srd 93	1115.00	-	6000.00	0.000
1351	CaBr2(cr)	tpis96	298.15	-	1015.00	-683.800
1352	CaBr2(L)	tpis96	1015.00	-	6000.00	-683.800
1353	CaCO3(cr)	tpis96	200.00	-	1603.00	-1206.600
1354	CaCO3(L)	tpis96	1603.00	-	6000.00	-1206.600
1355	CaCL2(cr)	tpis96	100.00	-	1048.00	-795.800
1356	CaCL2(L)	tpis96	1048.00	-	6000.00	-795.800
1357	CaF2(a)	tpis96	200.00	-	1424.00	-1228.000
1358	CaF2(b)	tpis96	1424.00	-	1691.00	-1228.000
1359	CaF2(L)	tpis96	1691.00	-	6000.00	-1228.000
1360	CaH2(a)	tpis96	298.15	-	1053.00	-177.000
1361	CaH2(b)	tpis96	1053.00	-	1273.00	-177.000
1362	CaH2(L)	tpis96	1273.00	-	6000.00	-177.000
1363	CaI2(cr)	tpis96	200.00	-	1056.00	-536.400
1364	CaI2(L)	tpis96	1056.00	-	6000.00	-536.400
1365	CaO(cr)	tpis96	200.00	-	3172.00	-634.920
1366	CaO(L)	tpis96	3172.00	-	6000.00	-634.920
1367	Ca(OH)2(cr)	tpis96	100.00	-	1023.00	-985.900
1368	Ca(OH)2(L)	tpis96	1023.00	-	6000.00	-985.900
1369	CaS(cr)	tpis96	200.00	-	2800.00	-475.000
1370	CaS(L)	tpis96	2800.00	-	6000.00	-475.000
1371	CaSO4(II)	tpis96	200.00	-	1473.00	-1434.000
1372	CaSO4(I)	tpis96	1473.00	-	1733.00	-1434.000
1373	CaSO4(L)	tpis96	1733.00	-	6000.00	-1434.000
1374	Cd(cr)	coda89	100.00	-	594.26	0.000
1375	Cd(L)	coda89	594.26	-	6000.00	0.000
1376	Co(a)	j 9/67	200.00	-	700.10	0.000
1377	Co(b)	j 9/67	700.10	-	1394.00	0.000
1378	Co(b)	j 9/67	1394.00	-	1768.00	0.000
1379	Co(L)	j 9/67	1768.00	-	6000.00	0.000
1380	Cr(cr)	j 6/73	200.00	-	311.50	0.000
1381	Cr(cr)	j 6/73	311.50	-	2130.00	0.000
1382	Cr(L)	j 6/73	2130.00	-	6000.00	0.000
1383	CrN(cr)	j12/73	200.00	-	2500.00	-117.152
1384	Cr2N(cr)	j12/73	298.15	-	2500.00	-125.520
1385	Cr2O3(I')	tpis82	200.00	-	306.00	-1140.600
1386	Cr2O3(I)	tpis82	306.00	-	310.00	-1140.600
1387	Cr2O3(I)	tpis82	310.00	-	335.00	-1140.600
1388	Cr2O3(I)	tpis82	335.00	-	2705.00	-1140.600
1389	Cr2O3(L)	tpis82	2705.00	-	6000.00	-1140.600
1390	Cs(cr)	coda89	100.00	-	301.59	0.000
1391	Cs(L)	coda89	301.59	-	2000.00	0.000
1392	CsBO2(cr)	tpis82	200.00	-	1005.00	-962.000
1393	CsBO2(L)	tpis82	1005.00	-	6000.00	-962.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1394	CsBr(cr)	tpis82	200.00 - 910.00	-405.600
1395	CsBr(L)	tpis82	910.00 - 6000.00	-405.600
1396	CsCL(a)	tpis82	200.00 - 743.00	-442.310
1397	CsCL(b)	tpis82	743.00 - 919.00	-442.310
1398	CsCL(L)	tpis82	919.00 - 6000.00	-442.310
1399	CsF(cr)	tpis82	200.00 - 976.00	-557.100
1400	CsF(L)	tpis82	976.00 - 6000.00	-557.100
1401	CsH(cr)	tpis82	298.15 - 801.00	-54.040
1402	CsH(L)	tpis82	801.00 - 6000.00	-54.040
1403	CsI(cr)	tpis82	200.00 - 905.00	-348.100
1404	CsI(L)	tpis82	905.00 - 6000.00	-348.100
1405	CsOH(b)	g 8/97	100.00 - 498.20	-416.200
1406	CsNO2(I)	tpis82	298.15 - 679.00	-379.900
1407	CsNO2(L)	tpis82	679.00 - 6000.00	-379.900
1408	CsNO3(a)	tpis82	200.00 - 427.00	-505.000
1409	CsNO3(b)	tpis82	427.00 - 682.00	-505.000
1410	CsNO3(L)	tpis82	682.00 - 6000.00	-505.000
1411	CsOH(c)	g 8/97	498.20 - 615.50	-416.200
1412	CsOH(L)	g 8/97	615.50 - 6000.00	-416.200
1413	CsO2(a)	tpis82	298.15 - 403.00	-286.100
1414	CsO2(c)	tpis82	403.00 - 723.00	-286.100
1415	CsO2(L)	tpis82	723.00 - 6000.00	-286.100
1416	Cs2CO3(cr)	tpis82	200.00 - 1066.00	-1134.900
1417	Cs2CO3(L)	tpis82	1066.00 - 6000.00	-1134.900
1418	Cs2O(cr)	tpis82	200.00 - 768.00	-346.400
1419	Cs2O(L)	tpis82	768.00 - 6000.00	-346.400
1420	Cs2O2(cr)	tpis82	298.15 - 867.00	-440.000
1421	Cs2O2(L)	tpis82	867.00 - 6000.00	-440.000
1422	Cs2SO4(a)	tpis82	200.00 - 920.00	-1442.900
1423	Cs2SO4(b)	tpis82	920.00 - 1000.00	-1442.900
1424	Cs2SO4(c)	tpis82	1000.00 - 1288.00	-1442.900
1425	Cs2SO4(L)	tpis82	1288.00 - 6000.00	-1442.900
1426	Cu(cr)	coda89	200.00 - 1358.00	0.000
1427	Cu(L)	coda89	1358.00 - 6000.00	0.000
1428	CuBr(a)	g10/00	298.15 - 657.00	-105.604
1429	CuBr(b)	g10/00	657.00 - 741.00	-105.604
1430	CuBr(c)	g10/00	741.00 - 759.00	-105.604
1431	CuBr(L)	g10/00	759.00 - 1500.00	-105.604
1432	CuBr2(cr)	g10/00	298.15 - 800.00	-138.490
1433	CuCL(a)	g10/00	298.15 - 685.00	-155.645
1434	CuCL(b)	g10/00	685.00 - 696.00	-155.645
1435	CuCL(L)	g10/00	696.00 - 1700.00	-155.645
1436	CuCL2(cr)	g10/00	298.15 - 675.00	-217.986
1437	CuCL2(L)	g10/00	675.00 - 6000.00	-217.986
1438	CuF(cr)	g10/00	298.15 - 1300.00	-209.200
1439	CuF2(cr)	g10/00	298.15 - 1109.00	-539.820
1440	CuF2(L)	g10/00	1109.00 - 6000.00	-539.820
1441	CuI(a)	g11/00	200.00 - 642.00	-67.781
1442	CuI(b)	g11/00	642.00 - 680.00	-67.781
1443	CuI(c)	g11/00	680.00 - 868.00	-67.781
1444	CuI(L)	g11/00	868.00 - 1600.00	-67.781
1445	CuO(cr)	g11/00	200.00 - 1400.00	-155.645
1446	Cu(OH)2(cr)	g10/00	298.15 - 2000.00	-443.086
1447	CuS(cr)	g10/00	298.15 - 717.82	-55.647

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^\circ(298.15)$
1448	CuSO4(cr)	g10/00	200.00 - 1500.00	-768.601
1449	Cu2O(cr)	g10/00	200.00 - 1516.70	-170.707
1450	Cu2O(L)	g10/00	1516.70 - 6000.00	-170.707
1451	Cu2S(a)	g10/00	298.15 - 376.00	-75.730
1452	Cu2S(b)	g10/00	376.00 - 720.00	-75.730
1453	Cu2S(c)	g10/00	720.00 - 1400.00	-75.730
1454	Cu2S(L)	g10/00	1400.00 - 6000.00	-75.730
1455	Fe(a)	j 3/78	200.00 - 1042.00	0.000
1456	Fe(a)	j 3/78	1042.00 - 1184.00	0.000
1457	Fe(c)	j 3/78	1184.00 - 1665.00	0.000
1458	Fe(d)	j 3/78	1665.00 - 1809.00	0.000
1459	Fe(L)	j 3/78	1809.00 - 6000.00	0.000
1460	Fe(CO)5(L)	j 3/78	253.10 - 6000.00	-766.090
1461	FeCL2(cr)	j12/70	200.00 - 950.00	-341.833
1462	FeCL2(L)	j12/70	950.00 - 6000.00	-341.833
1463	FeCL3(cr)	g12/00	200.00 - 577.00	-399.237
1464	FeCL3(L)	g12/00	577.00 - 6000.00	-399.237
1465	Fe.947O(cr)	g11/00	298.15 - 1652.00	-266.270
1466	Fe.947O(L)	g11/00	1652.00 - 6000.00	-266.270
1467	FeOCL(cr)	g12/00	200.00 - 700.00	-410.994
1468	Fe(OH)2(cr)	j 6/66	298.15 - 1500.00	-574.045
1469	Fe(OH)3(cr)	j 6/66	298.15 - 1500.00	-832.616
1470	FeS(a)	g11/00	200.00 - 411.00	-99.621
1471	FeS(b)	g11/00	411.00 - 598.00	-99.621
1472	FeS(c)	g11/00	598.00 - 1465.00	-99.621
1473	FeS(L)	g11/00	1465.00 - 6000.00	-99.621
1474	FeSO4(cr)	j 6/66	200.00 - 2000.00	-928.848
1475	FeS2(cr)	j 9/77	200.00 - 1400.00	-171.544
1476	Fe2O3(cr)	g 1/01	298.15 - 960.00	-824.248
1477	Fe2O3(cr)	g 1/01	960.00 - 6000.00	-824.248
1478	Fe2(SO4)3(cr)	j 6/66	298.15 - 2000.00	-2582.992
1479	Fe3O4(cr)	g 1/01	200.00 - 850.00	-1118.383
1480	Fe3O4(cr)	g 1/01	850.00 - 1870.00	-1118.383
1481	Fe3O4(L)	g 1/01	1870.00 - 6000.00	-1118.383
1482	Ga(cr)	tpis96	100.00 - 302.92	0.000
1483	Ga(L)	tpis96	302.92 - 6000.00	0.000
1484	GaBr3(cr)	tpis96	298.15 - 397.00	-387.000
1485	GaBr3(L)	tpis96	397.00 - 6000.00	-387.000
1486	GaCL3(cr)	tpis96	298.15 - 351.00	-527.000
1487	GaCL3(L)	tpis96	351.00 - 6000.00	-527.000
1488	GaF3(cr)	tpis96	298.15 - 2000.00	-1175.000
1489	GaI3(cr)	tpis96	298.15 - 485.00	-218.000
1490	GaI3(L)	tpis96	485.00 - 6000.00	-218.000
1491	Ga2O3(cr)	tpis96	200.00 - 2080.00	-1091.000
1492	Ga2O3(L)	tpis96	2080.00 - 6000.00	-1091.000
1493	Ge(cr)	tpis91	200.00 - 1211.40	0.000
1494	Ge(L)	tpis91	1211.40 - 6000.00	0.000
1495	GeO2(II)	tpis91	100.00 - 1308.00	-580.200
1496	GeO2(I)	tpis91	1308.00 - 1388.00	-580.200
1497	GeO2(L)	tpis91	1388.00 - 6000.00	-580.200
1498	GeS(II)	tpis91	100.00 - 931.00	-75.348
1499	GeS(L)	tpis91	931.00 - 6000.00	-75.348
1500	GeS(cr)	tpis91	100.00 - 931.00	-75.348
1501	GeS(L)	tpis91	931.00 - 6000.00	-75.348

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1502	GeS2(II)	tpis91	100.00 - 1113.00	-121.500
1503	GeS2(L)	tpis91	1113.00 - 6000.00	-121.500
1504	GeS2(cr)	tpis91	100.00 - 1113.00	-121.500
1505	GeS2(L)	tpis91	1113.00 - 6000.00	-121.500
1506	HBO2(cr)	tpis96	298.15 - 509.00	-804.600
1507	HBO2(L)	tpis96	509.00 - 6000.00	-804.600
1508	H2O(cr)	g11/99	200.00 - 273.15	-299.108
1509	H2O(L)	g11/99	273.15 - 600.00	-285.830
1510	H2SO4(L)	j 9/77	283.46 - 1000.00	-813.989
1511	H3BO3(cr)	tpis96	200.00 - 444.10	-1094.800
1512	H3BO3(L)	tpis96	444.10 - 6000.00	-1094.800
1513	H3PO4(cr)	j12/71	200.00 - 315.50	-1284.488
1514	H3PO4(L)	j12/71	315.50 - 1000.00	-1284.488
1515	Hg(cr)	j12/61	100.00 - 234.29	0.000
1516	Hg(L)	j12/61	234.29 - 2000.00	0.000
1517	HgBr2(cr)	j 3/62	298.15 - 514.00	-175.310
1518	HgBr2(L)	j 3/62	514.00 - 6000.00	-175.310
1519	HgO(cr)	j 6/62	200.00 - 1000.00	-90.789
1520	I2(cr)	tpis89	200.00 - 386.75	0.000
1521	I2(L)	tpis89	386.75 - 6000.00	0.000
1522	In(cr)	tpis96	100.00 - 429.78	0.000
1523	In(L)	tpis96	429.78 - 6000.00	0.000
1524	InBr(cr)	tpis96	298.15 - 558.00	-175.000
1525	InBr(L)	tpis96	558.00 - 6000.00	-175.000
1526	InBr3(cr)	tpis96	298.15 - 693.00	-399.000
1527	InBr3(L)	tpis96	693.00 - 6000.00	-399.000
1528	InCL(crII)	tpis96	298.15 - 387.00	-186.500
1529	InCL(crI)	tpis96	387.00 - 484.00	-186.500
1530	InCL(L)	tpis96	484.00 - 6000.00	-186.500
1531	InCl3(cr)	tpis96	298.15 - 856.00	-530.000
1532	InCl3(L)	tpis96	856.00 - 6000.00	-530.000
1533	InF3(cr)	tpis96	298.15 - 1445.00	-1190.000
1534	InF3(L)	tpis96	1445.00 - 6000.00	-1190.000
1535	InI(cr)	tpis96	200.00 - 637.50	-102.500
1536	InI(L)	tpis96	637.50 - 6000.00	-102.500
1537	InI2(crII)	tpis96	200.00 - 428.00	-176.000
1538	InI2(crI)	tpis96	428.00 - 497.00	-176.000
1539	InI2(L)	tpis96	497.00 - 6000.00	-176.000
1540	InI3(cr)	tpis96	296.00 - 480.00	-224.000
1541	InI3(L)	tpis96	480.00 - 6000.00	-224.000
1542	In2O3(cr)	tpis96	200.00 - 2186.00	-923.000
1543	In2O3(L)	tpis96	2186.00 - 6000.00	-923.000
1544	K(cr)	coda89	200.00 - 336.86	0.000
1545	K(L)	coda89	336.86 - 2200.00	0.000
1546	KALO2(II)	tpis82	200.00 - 810.00	-1130.600
1547	KALO2(I)	tpis82	810.00 - 1986.00	-1130.600
1548	KALO2(L)	tpis82	1986.00 - 6000.00	-1130.600
1549	KBO2(cr)	tpis82	200.00 - 1220.00	-983.000
1550	KBO2(L)	tpis82	1220.00 - 6000.00	-983.000
1551	KBr(cr)	tpis82	200.00 - 1007.00	-393.450
1552	KBr(L)	tpis82	1007.00 - 6000.00	-393.450
1553	KCN(II)	j 3/66	168.30 - 895.00	-113.470
1554	KCN(L)	j 3/66	895.00 - 6000.00	-113.470
1555	KCL(cr)	tpis82	200.00 - 1044.00	-436.490

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1556	KCL(L)	tpis82	1044.00 - 6000.00	-436.490
1557	KF(cr)	tpis82	200.00 - 1131.00	-569.900
1558	KF(L)	tpis82	1131.00 - 6000.00	-569.900
1559	KH(cr)	tpis82	298.15 - 892.00	-57.820
1560	KH(L)	tpis82	892.00 - 6000.00	-57.820
1561	K(HF2)(a)	j 6/71	200.00 - 469.85	-931.233
1562	K(HF2)(b)	j 6/71	469.85 - 511.95	-931.233
1563	K(HF2)(L)	j 6/71	511.95 - 6000.00	-931.233
1564	KI(cr)	tpis82	200.00 - 954.00	-329.300
1565	KI(L)	tpis82	954.00 - 6000.00	-329.300
1566	KNO2(II)	tpis82	200.00 - 314.70	-365.900
1567	KNO2(I)	tpis82	314.70 - 711.00	-365.900
1568	KNO2(L)	tpis82	711.00 - 6000.00	-365.900
1569	KNO3(a)	tpis82	200.00 - 402.00	-494.000
1570	KNO3(b)	tpis82	402.00 - 607.70	-494.000
1571	KNO3(L)	tpis82	607.70 - 6000.00	-494.000
1572	KOH(a)	g 8/97	100.00 - 298.15	-423.400
1573	KOH(b)	g 8/97	298.15 - 517.00	-423.400
1574	KOH(c)	g 8/97	517.00 - 679.00	-423.400
1575	KOH(L)	g 8/97	679.00 - 6000.00	-423.400
1576	KO2(b)	tpis82	200.00 - 422.00	-283.600
1577	KO2(a)	tpis82	422.00 - 808.00	-283.600
1578	KO2(L)	tpis82	808.00 - 6000.00	-283.600
1579	K2CO3(a)	tpis82	200.00 - 693.00	-1151.500
1580	K2CO3(b)	tpis82	693.00 - 1173.00	-1151.500
1581	K2CO3(L)	tpis82	1173.00 - 6000.00	-1151.500
1582	K2O(c)	tpis82	298.15 - 590.00	-361.700
1583	K2O(b)	tpis82	590.00 - 645.00	-361.700
1584	K2O(a)	tpis82	645.00 - 1013.00	-361.700
1585	K2O(L)	tpis82	1013.00 - 6000.00	-361.700
1586	K2O2(cr)	tpis82	298.15 - 818.00	-443.000
1587	K2O2(L)	tpis82	818.00 - 6000.00	-443.000
1588	K2S(cr)	j 3/78	298.15 - 1050.00	-376.560
1589	K2S(cr)	j 3/78	1050.00 - 1221.00	-376.560
1590	K2S(L)	j 3/78	1221.00 - 6000.00	-376.560
1591	K2SO4(II)	tpis82	200.00 - 857.00	-1437.700
1592	K2SO4(I)	tpis82	857.00 - 1342.00	-1437.700
1593	K2SO4(L)	tpis82	1342.00 - 6000.00	-1437.700
1594	K2SiO3(cr)	tpis82	200.00 - 1249.00	-1543.000
1595	K2SiO3(L)	tpis82	1249.00 - 6000.00	-1543.000
1596	K2Si2O5(a)	tpis82	200.00 - 510.00	-2505.000
1597	K2Si2O5(b)	tpis82	510.00 - 867.00	-2505.000
1598	K2Si2O5(c)	tpis82	867.00 - 1318.00	-2505.000
1599	K2Si2O5(L)	tpis82	1318.00 - 6000.00	-2505.000
1600	K3ALF6(II)	tpis82	298.15 - 600.00	-3347.000
1601	K3ALF6(I)	tpis82	600.00 - 1273.00	-3347.000
1602	K3ALF6(L)	tpis82	1273.00 - 6000.00	-3347.000
1603	Li(cr)	tpis82	200.00 - 453.69	0.000
1604	Li(L)	tpis82	453.69 - 6000.00	0.000
1605	LiALO2(cr)	j12/79	200.00 - 1973.00	-1188.674
1606	LiALO2(L)	j12/79	1973.00 - 6000.00	-1188.674
1607	LiBO2(cr)	tpis82	200.00 - 1122.00	-1022.900
1608	LiBO2(L)	tpis82	1122.00 - 6000.00	-1022.900
1609	LiBr(cr)	tpis82	200.00 - 823.00	-351.160

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1610	LiBr(L)	tpis82	823.00 - 6000.00	-351.160
1611	LiCL(cr)	tpis82	200.00 - 883.00	-408.540
1612	LiCL(L)	tpis82	883.00 - 6000.00	-408.540
1613	LiF(cr)	tpis82	200.00 - 1122.00	-618.300
1614	LiF(L)	tpis82	1122.00 - 6000.00	-618.300
1615	LiH(cr)	tpis82	200.00 - 965.00	-90.650
1616	LiH(L)	tpis82	965.00 - 6000.00	-90.650
1617	LiI(cr)	tpis82	200.00 - 742.00	-273.200
1618	LiI(L)	tpis82	742.00 - 6000.00	-273.200
1619	LiNO2(II)	tpis82	298.15 - 369.00	-368.300
1620	LiNO2(I)	tpis82	369.00 - 495.00	-368.300
1621	LiNO2(L)	tpis82	495.00 - 6000.00	-368.300
1622	LiNO3(cr)	tpis82	298.15 - 526.00	-482.700
1623	LiNO3(L)	tpis82	525.00 - 6000.00	-482.700
1624	LiOH(cr)	g 9/99	200.00 - 746.00	-487.500
1625	LiOH(L)	g 9/99	746.00 - 6000.00	-487.500
1626	Li2CO3(cr)	tpis82	200.00 - 1005.00	-1214.100
1627	Li2CO3(L)	tpis82	1005.00 - 6000.00	-1214.100
1628	Li2O(cr)	tpis82	200.00 - 1726.00	-597.880
1629	Li2O(L)	tpis82	1726.00 - 6000.00	-597.880
1630	Li2O2(cr)	tpis82	298.15 - 1000.00	-632.500
1631	Li2SO4(a)	tpis82	200.00 - 848.00	-1436.000
1632	Li2SO4(b)	tpis82	848.00 - 1131.00	-1436.000
1633	Li2SO4(L)	tpis82	1131.00 - 6000.00	-1436.000
1634	Li3ALF6(IV)	tpis82	200.00 - 788.00	-3389.600
1635	Li3ALF6(III)	tpis82	788.00 - 873.00	-3389.600
1636	Li3ALF6(II)	tpis82	873.00 - 978.00	-3389.600
1637	Li3ALF6(I)	tpis82	978.00 - 1058.00	-3389.600
1638	Li3ALF6(L)	tpis82	1058.00 - 6000.00	-3389.600
1639	Li3N(cr)	j 3/78	200.00 - 1300.00	-164.557
1640	Mg(cr)	srd 93	100.00 - 923.00	0.000
1641	Mg(L)	srd 93	923.00 - 6000.00	0.000
1642	MgAL2O4(cr)	j12/79	200.00 - 2408.00	-2299.110
1643	MgAL2O4(L)	j12/79	2408.00 - 6000.00	-2299.110
1644	MgBr2(cr)	tpis96	298.15 - 984.00	-526.000
1645	MgBr2(L)	tpis96	984.00 - 6000.00	-526.000
1646	MgCO3(cr)	tpis96	200.00 - 1263.00	-1096.000
1647	MgCO3(L)	tpis96	1263.00 - 6000.00	-1096.000
1648	MgCL2(cr)	tpis96	200.00 - 987.00	-644.300
1649	MgCL2(L)	tpis96	987.00 - 6000.00	-644.300
1650	MgF2(cr)	tpis96	200.00 - 1536.00	-1124.200
1651	MgF2(L)	tpis96	1536.00 - 6000.00	-1124.200
1652	MgH2(b)	tpis96	200.00 - 600.00	-75.700
1653	MgH2(L)	tpis96	600.00 - 6000.00	-75.700
1654	MgI2(cr)	tpis96	298.15 - 906.00	-370.000
1655	MgI2(L)	tpis96	906.00 - 6000.00	-370.000
1656	MgO(cr)	tpis96	200.00 - 3100.00	-601.600
1657	MgO(L)	tpis96	3100.00 - 6000.00	-601.600
1658	Mg(OH)2(cr)	tpis96	200.00 - 1000.00	-924.350
1659	Mg(OH)2(L)	tpis96	1100.00 - 6000.00	-924.350
1660	MgS(cr)	tpis96	200.00 - 2500.00	-348.000
1661	MgS(L)	tpis96	2500.00 - 6000.00	-348.000
1662	MgSO4(II)	tpis96	200.00 - 1283.00	-1288.800
1663	MgSO4(I)	tpis96	1283.00 - 1410.00	-1288.800

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range			$\Delta_f H^o$(298.15)
1664	MgSO4(L)	tpis96	1410.00	-	6000.00	-1288.800
1665	MgSiO3(I)	j12/67	200.00	-	903.00	-1548.917
1666	MgSiO3(II)	j12/67	903.00	-	1258.00	-1548.917
1667	MgSiO3(III)	j12/67	1258.00	-	1850.00	-1548.917
1668	MgSiO3(L)	j12/67	1850.00	-	6000.00	-1548.917
1669	MgTiO3(cr)	j 6/67	200.00	-	1953.00	-1572.556
1670	MgTiO3(L)	j 6/67	1953.00	-	6000.00	-1572.556
1671	MgTi2O5(cr)	g11/00	200.00	-	1963.00	-2508.219
1672	MgTi2O5(L)	g11/00	1963.00	-	6000.00	-2508.219
1673	Mg2SiO4(cr)	g11/00	200.00	-	2171.00	-2177.078
1674	Mg2SiO4(L)	g11/00	2170.00	-	6000.00	-2177.078
1675	Mg2TiO4(cr)	g11/00	200.00	-	2013.00	-2164.354
1676	Mg2TiO4(L)	g11/00	2013.00	-	6000.00	-2164.354
1677	Mg3N2(cr)	tpis96	298.15	-	6000.00	-461.300
1678	Mn(a)	j 9/67	200.00	-	980.00	0.000
1679	Mn(b)	j 9/67	980.00	-	1361.00	0.000
1680	Mn(c)	j 9/67	1361.00	-	1412.00	0.000
1681	Mn(d)	j 9/67	1412.00	-	1519.00	0.000
1682	Mn(L)	j 9/67	1519.00	-	6000.00	0.000
1683	Mo(cr)	j 3/78	200.00	-	2896.00	0.000
1684	Mo(L)	j 3/78	2896.00	-	6000.00	0.000
1685	MoO2(cr)	tpis82	200.00	-	6000.00	-589.300
1686	MoO3(cr)	tpis82	200.00	-	1075.00	-744.600
1687	MoO3(L)	tpis82	1075.00	-	6000.00	-744.600
1688	NH4CL(II)	j 9/65	298.15	-	457.70	-314.553
1689	NH4CL(III)	j 9/65	457.70	-	1500.00	-314.553
1690	NH4F(cr)	tpis89	200.00	-	511.00	-467.560
1691	NH4F(L)	tpis89	511.00	-	6000.00	-467.560
1692	Na(cr)	coda89	200.00	-	371.01	0.000
1693	Na(L)	coda89	371.01	-	2300.00	0.000
1694	NaALO2(a)	j 3/63	200.00	-	740.00	-1133.190
1695	NaALO2(b)	j 3/63	740.00	-	3000.00	-1133.190
1696	NaBO2(cr)	tpis82	200.00	-	1239.00	-976.500
1697	NaBO2(L)	tpis82	1239.00	-	6000.00	-976.500
1698	NaBr(cr)	tpis82	200.00	-	1020.00	-361.160
1699	NaBr(L)	tpis82	1020.00	-	6000.00	-361.160
1700	NaCN(II)	g 8/01	197.70	-	288.50	-90.709
1701	NaCN(III)	g 8/01	288.50	-	835.00	-90.709
1702	NaCN(L)	g 8/01	835.00	-	6000.00	-90.709
1703	NaCL(cr)	tpis82	200.00	-	1074.00	-411.260
1704	NaCL(L)	tpis82	1074.00	-	6000.00	-411.260
1705	NaF(cr)	tpis82	200.00	-	1269.00	-576.600
1706	NaF(L)	tpis82	1269.00	-	6000.00	-576.600
1707	NaH(cr)	tpis82	200.00	-	911.00	-56.380
1708	NaH(L)	tpis82	911.00	-	6000.00	-56.380
1709	NaI(cr)	tpis82	200.00	-	934.00	-289.630
1710	NaI(L)	tpis82	934.00	-	6000.00	-289.630
1711	NaNO2(I)	tpis82	298.15	-	436.70	-354.600
1712	NaNO2(I')	tpis82	436.70	-	557.00	-354.600
1713	NaNO2(L)	tpis82	557.00	-	6000.00	-354.600
1714	NaNO3(a)	tpis82	200.00	-	549.00	-467.700
1715	NaNO3(b)	tpis82	549.00	-	579.60	-467.700
1716	NaNO3(L)	tpis82	579.60	-	6000.00	-467.700
1717	NaOH(a)	g 5/99	100.00	-	514.00	-425.800

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1718	NaOH(b)	g 5/99	514.00 - 568.00	-425.800
1719	NaOH(c)	g 5/99	568.00 - 594.00	-425.800
1720	NaOH(L)	g 5/99	594.00 - 6000.00	-425.800
1721	NaO2(cr)	g10/99	223.30 - 825.00	-261.000
1722	NaO2(L)	g10/99	825.00 - 6000.00	-261.000
1723	Na2CO3(a)	tpis82	200.00 - 623.00	-1129.190
1724	Na2CO3(b)	tpis82	623.00 - 752.00	-1129.190
1725	Na2CO3(c)	tpis82	752.00 - 1131.00	-1129.190
1726	Na2CO3(L)	tpis82	1131.00 - 6000.00	-1129.190
1727	Na2O(c)	tpis82	200.00 - 1023.00	-414.570
1728	Na2O(b)	tpis82	1023.00 - 1243.00	-414.570
1729	Na2O(a)	tpis82	1243.00 - 1405.00	-414.570
1730	Na2O(L)	tpis82	1405.00 - 6000.00	-414.570
1731	Na2O2(b)	tpis82	200.00 - 785.00	-512.000
1732	Na2O2(a)	tpis82	785.00 - 948.00	-512.000
1733	Na2O2(L)	tpis82	948.00 - 6000.00	-512.000
1734	Na2S(cr)	j 3/78	298.15 - 1276.00	-366.100
1735	Na2S(cr)	j 3/78	1276.00 - 1445.00	-366.100
1736	Na2S(L)	j 3/78	1445.00 - 6000.00	-366.100
1737	Na2SO3(s)	bar 89	298.15 - 1184.00	-1100.802
1738	Na2SO3(L)	bar 89	1184.00 - 6000.00	-1100.802
1739	Na2SO4(V)	tpis82	200.00 - 458.00	-1387.900
1740	Na2SO4(IV)	tpis82	458.00 - 514.00	-1387.900
1741	Na2SO4(I)	tpis82	514.00 - 1157.00	-1387.900
1742	Na2SO4(L)	tpis82	1157.00 - 6000.00	-1387.900
1743	Na3ALF6(a)	tpis82	200.00 - 838.00	-3322.400
1744	Na3ALF6(b)	tpis82	838.00 - 1286.00	-3322.400
1745	Na3ALF6(L)	tpis82	1286.00 - 6000.00	-3322.400
1746	Na5AL3F14(cr)	tpis82	200.00 - 1010.00	-7555.000
1747	Na5AL3F14(L)	tpis82	1010.00 - 6000.00	-7555.000
1748	Nb(cr)	j12/73	200.00 - 2750.00	0.000
1749	Nb(L)	j12/73	2750.00 - 6000.00	0.000
1750	NbO(cr)	tpis82	298.15 - 2217.00	-406.000
1751	NbO(L)	tpis82	2217.00 - 6000.00	-406.000
1752	NbOCL3(cr)	bar 89	298.15 - 702.00	-879.500
1753	NbO2(II)	tpis82	200.00 - 1082.00	-795.000
1754	NbO2(I)	tpis82	1082.00 - 2360.00	-795.000
1755	NbO2(L)	tpis82	2360.00 - 6000.00	-795.000
1756	Nb2O5(cr)	tpis82	200.00 - 1783.00	-1897.000
1757	Nb2O5(L)	tpis82	1783.00 - 6000.00	-1897.000
1758	Ni(cr)	j12/76	200.00 - 631.00	0.000
1759	Ni(cr)	j12/76	631.00 - 1728.00	0.000
1760	Ni(L)	j12/76	1728.00 - 6000.00	0.000
1761	NiS(b)	j12/76	200.00 - 652.00	-87.864
1762	NiS(a)	j12/76	652.00 - 1249.00	-87.864
1763	NiS(L)	j12/76	1249.00 - 6000.00	-87.864
1764	NiS2(cr)	j 3/77	298.15 - 1280.00	-131.378
1765	NiS2(L)	j 3/77	1280.00 - 6000.00	-131.378
1766	Ni3S2(a)	g12/00	200.00 - 834.00	-217.986
1767	Ni3S2(b)	g12/00	834.00 - 1064.00	-217.986
1768	Ni3S2(L)	g12/00	1064.00 - 6000.00	-217.986
1769	Ni3S4(cr)	j 3/77	298.15 - 1100.00	-301.115
1770	P(cr)	tpis89	195.40 - 317.30	0.000
1771	P(L)	tpis89	317.30 - 6000.00	0.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o$(298.15)
1772	P4O10(cr)	tpis89	100.00 - 699.00	-3010.100
1773	P4O10(L)	tpis89	699.00 - 6000.00	-3010.100
1774	Pb(cr)	tpis91	200.00 - 600.65	0.000
1775	Pb(L)	tpis91	600.65 - 3600.00	0.000
1776	PbBr2(s)	tpis91	100.00 - 644.00	-276.700
1777	PbBr2(L)	tpis91	644.00 - 6000.00	-276.700
1778	PbCL2(cr)	tpis91	200.00 - 774.00	-359.400
1779	PbCL2(L)	tpis91	774.00 - 6000.00	-359.400
1780	PbF2(II)	tpis91	298.15 - 583.00	-676.000
1781	PbF2(I)	tpis91	583.00 - 1103.00	-676.000
1782	PbF2(L)	tpis91	1103.00 - 6000.00	-676.000
1783	PbI2(s)	tpis91	100.00 - 683.00	-176.000
1784	PbI2(L)	tpis91	683.00 - 6000.00	-176.000
1785	PbO(II-r)	tpis91	100.00 - 762.00	-218.600
1786	PbO(I-y)	tpis91	762.00 - 1160.00	-218.600
1787	PbO(L)	tpis91	1160.00 - 6000.00	-218.600
1788	PbO2(s)	tpis91	100.00 - 1000.00	-276.000
1789	PbS(cr)	tpis91	100.00 - 1386.50	-99.475
1790	PbS(L)	tpis91	1386.50 - 6000.00	-99.475
1791	Pb2O3(s)	tpis91	100.00 - 1000.00	-491.700
1792	Pb3O4(cr)	tpis91	200.00 - 1000.00	-720.000
1793	Rb(cr)	coda89	100.00 - 312.47	0.000
1794	Rb(L)	coda89	312.47 - 2100.00	0.000
1795	RbBO2(b)	tpis82	200.00 - 968.00	-975.000
1796	RbBO2(a)	tpis82	968.00 - 1133.00	-975.000
1797	RbBO2(L)	tpis82	1133.00 - 6000.00	-975.000
1798	RbBr(cr)	tpis82	200.00 - 965.00	-394.770
1799	RbBr(L)	tpis82	965.00 - 6000.00	-394.770
1800	RbCL(cr)	tpis82	200.00 - 997.00	-435.220
1801	RbCL(L)	tpis82	997.00 - 6000.00	-435.220
1802	RbF(cr)	tpis82	298.15 - 1068.00	-559.700
1803	RbF(L)	tpis82	1068.00 - 6000.00	-559.700
1804	RbH(cr)	tpis82	298.15 - 858.00	-52.300
1805	RbH(L)	tpis82	858.00 - 6000.00	-52.300
1806	RbI(cr)	tpis82	200.00 - 929.00	-333.600
1807	RbI(L)	tpis82	929.00 - 6000.00	-333.600
1808	RbNO2(I)	tpis82	298.15 - 695.00	-367.000
1809	RbNO2(L)	tpis82	695.00 - 6000.00	-367.000
1810	RbNO3(IV)	tpis82	200.00 - 437.00	-494.700
1811	RbNO3(III)	tpis82	437.00 - 493.00	-494.700
1812	RbNO3(II)	tpis82	493.00 - 556.00	-494.700
1813	RbNO3(I)	tpis82	556.00 - 583.00	-494.700
1814	RbNO3(L)	tpis82	583.00 - 6000.00	-494.700
1815	RbOH(b)	g 8/97	298.15 - 508.00	-418.800
1816	RbOH(c)	g 8/97	508.00 - 658.00	-418.800
1817	RbOH(L)	g 8/97	658.00 - 6000.00	-418.800
1818	RbO2(b)	tpis82	200.00 - 423.00	-279.100
1819	RbO2(a)	tpis82	423.00 - 813.00	-279.100
1820	RbO2(L)	tpis82	813.00 - 6000.00	-279.100
1821	Rb2CO3(a)	tpis82	200.00 - 576.00	-1132.600
1822	Rb2CO3(b)	tpis82	576.00 - 1146.00	-1132.600
1823	Rb2CO3(L)	tpis82	1146.00 - 6000.00	-1132.600
1824	Rb2O(c)	tpis82	298.15 - 543.00	-338.000
1825	Rb2O(b)	tpis82	543.00 - 613.00	-338.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range			$\Delta_f H^o$(298.15)
1826	Rb2O(a)	tpis82	613.00	-	778.00	-338.000
1827	Rb2O(L)	tpis82	778.00	-	6000.00	-338.000
1828	Rb2O2(b)	tpis82	298.15	-	398.00	-410.000
1829	Rb2O2(a)	tpis82	398.00	-	843.00	-410.000
1830	Rb2O2(L)	tpis82	843.00	-	6000.00	-410.000
1831	Rb2SO4(a)	tpis82	200.00	-	800.00	-1435.900
1832	Rb2SO4(a)	tpis82	800.00	-	931.00	-1435.900
1833	Rb2SO4(b)	tpis82	931.00	-	1343.00	-1435.900
1834	Rb2SO4(L)	tpis82	1343.00	-	6000.00	-1435.900
1835	S(a)	tpis89	200.00	-	368.30	0.000
1836	S(b)	tpis89	368.30	-	388.36	0.000
1837	S(L)	tpis89	388.36	-	6000.00	0.000
1838	SCL2(L)	j 6/78	298.15	-	6000.00	-49.790
1839	S2CL2(L)	j 6/78	298.15	-	6000.00	-58.158
1840	Sc(a)	tpis82	100.00	-	1609.00	0.000
1841	Sc(b)	tpis82	1609.00	-	1814.00	0.000
1842	Sc(l)	tpis82	1814.00	-	6000.00	0.000
1843	Sc2O3(cr)	tpis82	200.00	-	2762.00	-1908.600
1844	Sc2O3(L)	tpis82	2762.00	-	6000.00	-1908.600
1845	Si(cr)	tpis91	200.00	-	1690.00	0.000
1846	Si(L)	tpis91	1690.00	-	6000.00	0.000
1847	SiC(b)	tpis91	100.00	-	3105.00	-73.000
1848	SiC(L)	tpis91	3103.00	-	6000.00	-73.000
1849	SiO2(a-qz)	tpis91	200.00	-	848.00	-910.700
1850	SiO2(b-qz)	tpis91	848.00	-	1200.00	-910.700
1851	SiO2(b-crt)	tpis91	1200.00	-	1996.00	-910.700
1852	SiO2(L)	tpis91	1996.00	-	6000.00	-910.700
1853	SiS(cr)	tpis91	298.15	-	1363.00	-168.737
1854	SiS(L)	tpis91	1363.00	-	6000.00	-168.737
1855	SiS2(cr)	tpis91	100.00	-	1363.00	-287.000
1856	SiS2(L)	tpis91	1363.00	-	6000.00	-287.000
1857	Si2N2O(cr)	g 7/95	298.15	-	2500.00	-947.700
1858	Si3N4(cr)	tpis91	100.00	-	4000.00	-787.800
1859	Sn(cr)	tpis91	200.00	-	505.12	0.000
1860	Sn(L)	tpis91	505.12	-	4700.00	0.000
1861	SnBr2(cr)	tpis91	100.00	-	503.40	-253.600
1862	SnBr2(L)	tpis91	503.40	-	6000.00	-253.600
1863	SnBr4(cr)	tpis91	200.00	-	302.25	-388.000
1864	SnBr4(L)	tpis91	302.25	-	6000.00	-388.000
1865	SnCL2(cr)	tpis91	200.00	-	520.20	-333.000
1866	SnCL2(L)	tpis91	520.20	-	6000.00	-333.000
1867	SnCL4(L)	tpis91	239.05	-	6000.00	-517.000
1868	SnF2(cr)	tpis91	298.15	-	488.20	-677.000
1869	SnF2(L)	tpis91	488.20	-	6000.00	-677.000
1870	SnI2(cr)	tpis91	200.00	-	595.70	-153.000
1871	SnI2(L)	tpis91	595.70	-	6000.00	-153.000
1872	SnI4(cr)	tpis91	200.00	-	418.00	-207.500
1873	SnI4(L)	tpis91	418.00	-	6000.00	-207.500
1874	SnO(cr)	tpis91	100.00	-	1250.00	-280.710
1875	SnO(L)	tpis91	1250.00	-	6000.00	-280.710
1876	SnO2(cr)	tpis91	100.00	-	1903.00	-577.630
1877	SnO2(L)	tpis91	1903.00	-	6000.00	-577.630
1878	SnS(rh)	tpis91	100.00	-	875.00	-109.662
1879	SnS(cu)	tpis91	875.00	-	1154.00	-109.662

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range	$\Delta_f H^o(298.15)$
1880	SnS(L)	tpis91	1154.00 - 6000.00	-109.662
1881	SnS2(cr)	tpis91	100.00 - 1143.00	-141.837
1882	Sr(a)	srd 93	100.00 - 820.00	0.000
1883	Sr(b)	srd 93	820.00 - 1041.00	0.000
1884	Sr(L)	srd 93	1041.00 - 6000.00	0.000
1885	SrBr2(a)	tpis96	200.00 - 918.00	-722.000
1886	SrBr2(b)	tpis96	918.00 - 930.00	-722.000
1887	SrBr2(L)	tpis96	930.00 - 6000.00	-722.000
1888	SrCO3(a)	tpis96	200.00 - 1198.00	-1226.000
1889	SrCO3(b)	tpis96	1198.00 - 1689.00	-1226.000
1890	SrCO3(c)	tpis96	1689.00 - 1767.00	-1226.000
1891	SrCO3(L)	tpis96	1767.00 - 6000.00	-1226.000
1892	SrCL2(a)	tpis96	200.00 - 990.00	-833.000
1893	SrCL2(b)	tpis96	900.00 - 1147.00	-833.000
1894	SrCL2(L)	tpis96	1147.00 - 6000.00	-833.000
1895	SrF2(a)	tpis96	200.00 - 1484.00	-1229.000
1896	SrF2(b)	tpis96	1484.00 - 1750.00	-1229.000
1897	SrF2(L)	tpis96	1750.00 - 6000.00	-1229.000
1898	SrH2(a)	tpis96	298.00 - 1128.00	-180.000
1899	SrH2(b)	tpis96	1128.00 - 1323.00	-180.000
1900	SrH2(L)	tpis96	1323.00 - 6000.00	-180.000
1901	SrI2(cr)	tpis96	200.00 - 811.00	-568.000
1902	SrI2(L)	tpis96	811.00 - 6000.00	-568.000
1903	SrO(cr)	tpis96	200.00 - 2805.00	-591.000
1904	SrO(L)	tpis96	2805.00 - 6000.00	-591.000
1905	Sr(OH)2(b)	tpis96	200.00 - 753.00	-964.300
1906	Sr(OH)2(a)	tpis96	753.00 - 808.00	-964.300
1907	Sr(OH)2(L)	tpis96	808.00 - 6000.00	-964.300
1908	SrS(cr)	tpis96	200.00 - 2500.00	-480.000
1909	SrS(L)	tpis96	2500.00 - 6000.00	-480.000
1910	SrS04(a)	tpis96	298.15 - 1430.00	-1457.000
1911	SrS04(b)	tpis96	1430.00 - 1880.00	-1457.000
1912	SrS04(L)	tpis96	1880.00 - 6000.00	-1457.000
1913	Ta(cr)	j12/72	200.00 - 3258.00	0.000
1914	Ta(L)	j12/72	3258.00 - 6000.00	0.000
1915	TaC(cr)	j12/73	200.00 - 4273.00	-144.097
1916	TaC(L)	j12/73	4273.00 - 6000.00	-144.097
1917	Ta2O5(II)	tpis82	200.00 - 1633.00	-2049.000
1918	Ta2O5(I)	tpis82	1633.00 - 2150.00	-2049.000
1919	Ta2O5(L)	tpis82	2150.00 - 6000.00	-2049.000
1920	Th(a)	coda89	200.00 - 1650.00	0.000
1921	Th(b)	coda89	1650.00 - 2023.00	0.000
1922	Th(L)	coda89	2023.00 - 6000.00	0.000
1923	Ti(a)	coda89	200.00 - 1156.00	0.000
1924	Ti(b)	coda89	1156.00 - 1944.00	0.000
1925	Ti(L)	coda89	1944.00 - 6000.00	0.000
1926	TiB(cr)	j 6/65	298.15 - 4000.00	-160.247
1927	TiB2(cr)	j 6/65	200.00 - 3193.00	-279.491
1928	TiB2(L)	j 6/65	3193.00 - 6000.00	-279.491
1929	TiC(cr)	j 6/68	200.00 - 3290.00	-184.096
1930	TiC(L)	j 6/68	3290.00 - 6000.00	-184.096
1931	TiCL2(cr)	j12/68	200.00 - 2000.00	-515.470
1932	TiCL3(cr)	j12/68	298.15 - 1500.00	-721.740
1933	TiCL4(L)	j12/67	249.05 - 2000.00	-804.165

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range			$\Delta_f H^o$(298.15)
1934	TiN(cr)	j 6/68	200.00	-	3220.00	-337.649
1935	TiN(L)	j 6/68	3220.00	-	6000.00	-337.649
1936	TiO(a)	tpis82	200.00	-	1265.00	-542.000
1937	TiO(b)	tpis82	1265.00	-	1810.00	-542.000
1938	TiO(c)	tpis82	1810.00	-	2030.00	-542.000
1939	TiO(L)	tpis82	2030.00	-	6000.00	-542.000
1940	TiO2(ru)	tpis82	200.00	-	2185.00	-944.000
1941	TiO2(L)	tpis82	2185.00	-	6000.00	-944.000
1942	Ti2O3(I)	tpis82	200.00	-	464.00	-1520.000
1943	Ti2O3(I')	tpis82	464.00	-	2110.00	-1520.000
1944	Ti2O3(L)	tpis82	2110.00	-	6000.00	-1520.000
1945	Ti3O5(a)	tpis82	200.00	-	448.00	-2457.000
1946	Ti3O5(b)	tpis82	448.00	-	2050.00	-2457.000
1947	Ti3O5(L)	tpis82	2050.00	-	6000.00	-2457.000
1948	Ti4O7(cr)	tpis82	200.00	-	1960.00	-3403.000
1949	Ti4O7(L)	tpis82	1960.00	-	6000.00	-3403.000
1950	U(a)	coda89	200.00	-	942.00	0.000
1951	U(b)	coda89	942.00	-	1049.00	0.000
1952	U(c)	coda89	1049.00	-	1408.00	0.000
1953	U(L)	coda89	1408.00	-	4000.00	0.000
1954	UF3(cr)	tpis82	298.15	-	1768.00	-1508.700
1955	UF3(L)	tpis82	1768.00	-	6000.00	-1508.700
1956	UF4(cr)	tpis82	200.00	-	1309.00	-1920.500
1957	UF4(L)	tpis82	1309.00	-	6000.00	-1920.500
1958	UF5(b)	tpis82	298.15	-	398.00	-2083.000
1959	UF5(a)	tpis82	398.00	-	621.00	-2083.000
1960	UF5(L)	tpis82	621.00	-	6000.00	-2083.000
1961	UF6(cr)	tpis82	100.00	-	337.21	-2197.700
1962	UF6(L)	tpis82	337.21	-	1000.00	-2197.700
1963	UO2(cr)	tpis82	200.00	-	3123.00	-1085.000
1964	UO2(L)	tpis82	3123.00	-	6000.00	-1085.000
1965	UO3(c)	tpis82	200.00	-	3000.00	-1223.800
1966	UO2F2(cr)	tpis82	200.00	-	2100.00	-1653.600
1967	U3O8(II)	tpis82	200.00	-	483.00	-3574.800
1968	U3O8(I)	tpis82	483.00	-	6000.00	-3574.800
1969	U4O9(III)	tpis82	298.15	-	348.00	-4512.000
1970	U4O9(II)	tpis82	348.00	-	1398.00	-4512.000
1971	U4O9(I)	tpis82	1398.00	-	6000.00	-4512.000
1972	V(cr)	j 6/73	200.00	-	2190.00	0.000
1973	V(L)	j 6/73	2190.00	-	6000.00	0.000
1974	VCL2(cr)	g10/00	298.00	-	1300.00	-451.872
1975	VCL3(cr)	g 8/00	298.00	-	1000.00	-581.116
1976	VN(cr)	j12/73	200.00	-	3500.00	-217.150
1977	VO(cr)	tpis82	200.00	-	2063.00	-430.800
1978	VO(L)	tpis82	2063.00	-	6000.00	-430.800
1979	V2O3(cr)	tpis82	200.00	-	2230.00	-1216.800
1980	V2O3(L)	tpis82	2230.00	-	6000.00	-1216.800
1981	V2O4(II)	tpis82	200.00	-	338.70	-1432.600
1982	V2O4(I)	tpis82	338.70	-	1818.00	-1432.600
1983	V2O4(L)	tpis82	1818.00	-	6000.00	-1432.600
1984	V2O5(cr)	tpis82	200.00	-	954.00	-1551.000
1985	V2O5(L)	tpis82	954.00	-	6000.00	-1551.000
1986	W(cr)	j 6/66	200.00	-	3680.00	0.000
1987	W(L)	j 6/66	3680.00	-	6000.00	0.000

Appendix A *(continued)*

No.	Species Name	Reference Code (see page 43)	Temperature Range			$\Delta_f H^\circ$(298.15)
1988	WC(cr)	bar 89	298.15	-	2500.00	-40.540
1989	WCL6(I)	j12/66	298.15	-	450.00	-593.710
1990	WCL6(II)	j12/66	450.00	-	503.00	-593.710
1991	WCL6(III)	j12/66	503.00	-	555.00	-593.710
1992	WCL6(L)	j12/66	555.00	-	6000.00	-593.710
1993	WOCL4(cr)	j 3/67	298.15	-	484.00	-671.114
1994	WOCL4(L)	j 3/67	484.00	-	6000.00	-671.114
1995	WO2(cr)	tpis82	100.00	-	298.15	-588.100
1996	WO2(cr)	tpis82	298.15	-	6000.00	-588.100
1997	WO2CL2(cr)	j 3/67	298.15	-	1000.00	-780.316
1998	WO3(crIII)	tpis82	100.00	-	325.00	-841.300
1999	WO3(crIII,II)	tpis82	325.00	-	1013.00	-841.300
2000	WO3(crI)	tpis82	1013.00	-	1747.00	-841.300
2001	WO3(L)	tpis82	1747.00	-	6000.00	-841.300
2002	Zn(cr)	coda89	200.00	-	692.73	0.000
2003	Zn(L)	coda89	692.73	-	6000.00	0.000
2004	ZnSO4(a)	j 3/79	200.00	-	540.00	-980.144
2005	ZnSO4(a')	j 3/79	540.00	-	1013.00	-980.144
2006	ZnSO4(b)	j 3/79	1013.00	-	6000.00	-980.144
2007	Zr(a)	j 6/79	200.00	-	1135.00	0.000
2008	Zr(b)	j 6/79	1135.00	-	2125.00	0.000
2009	Zr(L)	j 6/79	2125.00	-	6000.00	0.000
2010	ZrN(cr)	g11/00	200.00	-	3225.00	-371.238
2011	ZrN(L)	g11/00	3225.00	-	6000.00	-371.238
2012	ZrO2(III)	tpis82	200.00	-	1445.00	-1100.300
2013	ZrO2(II)	tpis82	1445.00	-	2620.00	-1100.300
2014	ZrO2(I)	tpis82	2620.00	-	2983.00	-1100.300
2015	ZrO2(L)	tpis82	2983.00	-	6000.00	-1100.300
2016	Air	g 9/95	200.00	-	6000.00	-0.126
2017	CH3OH(L)	n12/84	175.61	-	390.00	-238.910
2018	C2H5OH(L)	n12/84	159.00	-	390.00	-277.510
2019	C6H6(L)	n10/86	278.68	-	500.00	49.080
2020	C6H5NH2(L)	n12/88	267.13	-	460.00	31.500
2021	C6H14(L),n-hexa	n 4/85	177.86	-	300.00	-198.660
2022	C7H8(L)	n10/86	178.15	-	500.00	12.180
2023	C7H16(L),n-hept	n10/75	182.58	-	380.00	-224.350
2024	C8H18(L),n-octa	n10/76	216.37	-	310.00	-250.260
2025	C8H18(L),isooct	n10/76	165.79	-	380.00	-259.160
2026	CLO3F	g 5/95	200.00	-	6000.00	-23.800
2027	H2O2(L)	tpis89	272.74	-	6000.00	-187.780
2028	JP-10	g 3/01	200.00	-	6000.00	-86.812
2029	Jet-A(L)	g 2/96	220.00	-	550.00	-303.403
2030	Jet-A(g)	g 2/96	273.15	-	5000.00	-249.657
2031	NH4CLO4(I)	j12/62	100.00	-	513.15	-295.767
2032	NH4CLO4(II)	j12/62	513.15	-	1500.00	-295.767
2033	NH4NO3(IV)	tpis89	256.20	-	305.38	-365.600
2034	NH4NO3(III)	tpis89	305.38	-	357.25	-365.600
2035	NH4NO3(II)	tpis89	357.25	-	399.00	-365.600
2036	NH4NO3(I)	tpis89	399.00	-	442.85	-365.600
2037	NH4NO3(L)	tpis89	442.85	-	6000.00	-365.600
2038	N2H4(L)	g 2/95	100.00	-	800.00	50.380

Six−character reference−date codes:

Letter	Reference	Numbers
g	Glenn (Multiple references)	Month/year calculated
j	NIST−JANAF Thermochemical Tables (Chase 1998 JPCRD 1998 Monograph 9)	Month/year of table
tpis	Thermodynamic Properties of Individual Substances (Gurvich 1982,1989,1991,1996)	Year of volume
n	NIST-TRC Thermodynamic Tables	Month/year of table
bar	Barin 1989	Year of volume
coda	CODATA (Garvin 1987, Cox 1989)	Year of volume
srd	Standard Reference Data	Year of JPCRD journal

Appendix B
Contents of File “cap.elms”

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Ag(cr)            Silver Cubic. Ref-Elm. Cox,1989 p228.
 1 coda89 AG  1.00    0.00    0.00    0.00    0.00 1    107.86820          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
 2.091668120D-09-3.888924460D-13               -4.614014260D+03 5.074216040D+00
Ag(L)             Silver Liquid. Ref-Elm. Cox,1989 p228.
 1 coda89 AG  1.00    0.00    0.00    0.00    0.00 2    107.86820          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. Ref-Elm. Cox,1989 p217.
 1 coda89 AL  1.00    0.00    0.00    0.00    0.00 1     26.98154          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. Ref-Elm. Cox,1989 p217.
 1 coda89 AL  1.00    0.00    0.00    0.00    0.00 2     26.98154          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
Ar                Ref-Elm. Moore,1971.
 3 g 3/98 AR  1.00    0.00    0.00    0.00    0.00 0   39.9480000          0.000
    200.000  1000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0         6197.428
 2.500000000D+00 0.000000000D+00 0.000000000D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00 0.000000000D+00-7.453750000D+02 4.379674910D+00
   1000.000  6000.000 7 -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 0.000000000D+00-7.449939610D+02 4.379180110D+00
   6000.000 20000.000 7 -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 0.000000000D+00-5.078300340D+06 1.465298484D+03
B(b)              Beta. Ref-Elm. Chase,1998 p177. McBride,1993a.
 2 j 6/83 B   1.00    0.00    0.00    0.00    0.00 1     10.81100          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. Ref-Elm. Chase,1998 p177. McBride,1993a.
 1 j 6/83 B   1.00    0.00    0.00    0.00    0.00 2     10.81100          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
Ba(cr)            Crystal. Ref-Elm. Alcock,1993.
 2 srd 93 BA  1.00    0.00    0.00    0.00    0.00 1    137.32700          0.000
     80.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6906.992
-1.121413048D+03 0.000000000D+00 2.794031158D+00 3.089779193D-03-8.812305235D-06
 1.741533776D-08 0.000000000D+00               -9.306838000D+02-9.109787138D+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 2.037522355D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.174338100D+02-8.909706262D+00
Ba(L)             Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 BA  1.00    0.00    0.00    0.00    0.00 2    137.32700          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 4.810866786D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.920623810D+02-2.000275711D+01
Be(a)             Alpha. Ref-Elm. Alcock,1993.
 2 srd 93 BE  1.00    0.00    0.00    0.00    0.00 1      9.01218          0.000
    100.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
 3.532378938D+03 0.000000000D+00-1.827528020D+00 1.895481514D-02-2.121592253D-05
 0.000000000D+00 0.000000000D+00               -9.832146860D+01 6.866894114D+00
    298.150   1543.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         1942.068
-7.064757875D+04 0.000000000D+00 2.550360755D+00 6.848268870D-04 1.157013462D-07
 0.000000000D+00 0.000000000D+00               -1.028803669D+03-1.399471510D+01
Be(b)             Beta. Ref-Elm. Alcock,1993.
 1 srd 93 BE  1.00    0.00    0.00    0.00    0.00 2      9.01218          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 3.608150089D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -8.524497790D+02-2.002895768D+01
Be(L)             Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 BE  1.00    0.00    0.00    0.00    0.00 3      9.01218          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 3.545608821D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.074755804D+02-1.895341257D+01
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Br2(cr)           Rhombic. Gurvich,1989 pt2 p314. Chase,1998 p471 (6/82).
 1 g 8/01 BR  2.00    0.00    0.00    0.00    0.00 1    159.80800          0.000
    200.000    265.9007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24520.000
-5.550117110D+06 1.610953162D+05-1.913542203D+03 1.201711944D+01-4.170621540D-02
 7.615296370D-05-5.694588430D-08                -6.565415920D+05 9.135571000D+03
Br2(L)            Liq. Ref-Elm.Gurvich,1989 pt2p314. Chase,1998p471(6/82).
 2 g 8/01 BR  2.00    0.00    0.00    0.00    0.00 2    159.80800          0.000
    265.900    332.5037 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        24520.000
 5.661619720D+06-6.002788720D+04 3.963572800D+01 2.194289283D+00-1.209616100D-02
 2.608732123D-05-2.065978604D-08                3.167204530D+05-6.832596160D+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 9.056697268D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.699852754D+03-3.329354185D+01
C(gr)             Graphite. Ref-Elm. TRC(4/83) VC,UC,TC-1000-1002.
 3 n 4/83 C   1.00    0.00    0.00    0.00    0.00 1     12.01070          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+0
Ca(a)             Alpha. Ref-Elm. Alcock,1993.
 2 srd 93 CA  1.00    0.00    0.00    0.00    0.00 1     40.07800          0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5782.945
 2.209214594D+04 0.000000000D+00-2.387095323D+00 4.674833430D-02-1.481690580D-04
 1.686114356D-07 0.000000000D+00               -3.160902334D+02 9.998907900D+00
    298.150    716.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5782.945
 8.959632100D+03 0.000000000D+00 2.440591375D+00 1.722094077D-03 4.744000490D-07
 0.000000000D+00 0.000000000D+00               -7.783440840D+02-9.273708050D+00
Ca(b)             Beta. Ref-Elm. Alcock,1993.
 1 srd 93 CA  1.00    0.00    0.00    0.00    0.00 2     40.07800          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 5.701117685D+00-5.810564904D-03 4.022125176D-06
 0.000000000D+00 0.000000000D+00               -1.516788311D+03-2.607588230D+01
Ca(L)             Liquid. Ref-Elm. Alcock,1993.
 1 srd 93 CA  1.00    0.00    0.00    0.00    0.00 3     40.07800          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 4.570323447D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -9.822680100D+02-2.119893317D+01
Cd(cr)            Crystal. Ref-Elm. Cox,1989 p223.
 1 coda89 CD  1.00    0.00    0.00    0.00    0.00 1    112.41100          0.000
    100.000    594.2587 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6247.000
 1.375273221D+05-3.221590070D+03 3.121905502D+01-1.226136798D-01 2.838880568D-04
-3.286884020D-07 1.520469817D-10                1.302807037D+04-1.551324136D+02
Cd(L)             Liquid. Ref-Elm. Cox,1989 p223.
 1 coda89 CD  1.00    0.00    0.00    0.00    0.00 2    112.41100          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 3.596122922D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.220394750D+02-1.323298164D+01
CL2               Ref-Elm. Gurvich,1989 pt1 p177: pt2 p88.
 2 tpis89 CL  2.00    0.00    0.00    0.00    0.00 0     70.90540          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9181.110
 3.462815170D+04-5.547126520D+02 6.207589370D+00-2.989632078D-03 3.173027290D-06
-1.793629562D-09 4.260043590D-13                1.534069331D+03-9.438343800D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9181.110
 6.092569420D+06-1.949627662D+04 2.854535795D+01-1.449968764D-02 4.463890770D-06
-6.358525860D-10 3.327360290D-14                1.212117724D+05-1.690778951D+02
Co(a)             Alpha. Ref-Elm. Chase,1998 p943.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 1     58.93320          0.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
-8.651834510D+05 1.462135206D+04-9.971089110D+01 3.794338600D-01-7.800106350D-04
 8.553583960D-07-3.890151670D-10               -6.795963460D+04 5.306550210D+02
    500.000    700.1007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
-9.877560740D+05 6.820602200D+03-1.521637485D+01 2.234541680D-02-9.019246600D-06
 0.000000000D+00 0.000000000D+00               -3.852839040D+04 1.014399403D+02
Co(b)             Beta.Ref-Elm.Below Lambda trans. Chase,1998 p943.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 2     58.93320          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 2.125113886D+00 2.218475342D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -6.197709420D+02-8.944546990D+00
    800.000   1394.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
-1.576349295D+09 9.154318170D+06-2.197967504D+04 2.793356668D+01-1.980310380D-02
 7.425124740D-06-1.149433030D-09               -5.182198410D+07 1.399846247D+05
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Co(b)             Beta. Ref-Elm.Above Lambda trans. Chase,1998 p943.
 2 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 3     58.93320          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 3.070872109D+02-2.155487195D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.139292950D+05-1.913104819D+03
   1400.000   1768.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4771.000
 1.648338062D+09-4.036220190D+06 3.722685700D+03-1.526326566D+00 2.354674115D-04
 0.000000000D+00 0.000000000D+00                2.649010262D+07-2.751466647D+04
Co(L)             Liquid. Ref-Elm. Chase,1998 p943.
 1 j 9/67 CO  1.00    0.00    0.00    0.00    0.00 4     58.93320          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 4.871122892D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.761381676D+02-2.448402276D+01
Cr(cr)            Below lambda trans. Ref-Elm. Chase,1998 p959.
 1 j 6/73 CR  1.00    0.00    0.00    0.00    0.00 1     51.99610          0.000
    200.000    311.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4057.000
 8.051084050D+05-1.339842819D+04 8.273507290D+01-2.075857041D-01 2.008764131D-04
 0.000000000D+00 0.000000000D+00                6.182357950D+04-4.559971660D+02
Cr(cr)            Above lambda trans. Ref-Elm. Chase,1998 p959.
 2 j 6/73 CR  1.00    0.00    0.00    0.00    0.00 2     51.99610          0.000
    311.500   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4057.000
-2.534425357D+05 3.119404093D+03-1.358439770D+01 4.323570220D-02-5.624102820D-05
 3.652910710D-08-8.973298370D-12               -1.606559079D+04 7.858043710D+01
   1000.000   2130.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4057.000
-3.005006418D+07 1.264410306D+05-2.139399408D+02 1.937684814D-01-9.423205780D-05
 2.445139082D-08-2.606793685D-12               -7.582388710D+05 1.441907828D+03
Cr(L)             Liquid. Ref-Elm. Chase,1998 p959.
 1 j 6/73 CR  1.00    0.00    0.00    0.00    0.00 3     51.99610          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 4.730284767D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                5.755633080D+02-2.453179007D+01
Cs(cr)            Crystal. Ref-Elm. Cox,1989 p263.
 1 coda89 CS  1.00    0.00    0.00    0.00    0.00 1    132.90545          0.000
    100.000    301.5907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7711.000
 6.519841350D+04-1.756639077D+03 1.999681093D+01-6.938328820D-02 1.093682552D-04
 0.000000000D+00 0.000000000D+00                6.382890840D+03-9.338251570D+01
Cs(L)             Liquid. Ref-Elm. Cox,1989 p263.
 2 coda89 CS  1.00    0.00    0.00    0.00    0.00 2    132.90545          0.000
    301.590   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7711.000
-4.218078030D+04-1.745861711D+01 5.702246950D+00-5.113948550D-03 3.201752440D-06
-1.767959558D-10 4.827862700D-14               -1.290810964D+03-2.031478114D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7711.000
-7.255372990D+05 3.001930225D+03 1.782289032D-01 2.832281079D-04 1.810515176D-07
 7.718855550D-10-8.889289510D-14               -1.920877274D+04 1.635273378D+01
Cu(cr)            Cubic. Ref-Elm.Cox,1989 p226.
 1 coda89 CU  1.00    0.00    0.00    0.00    0.00 1     63.54600          0.000
    200.000   1358.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5004.000
-2.455775109D+04 1.648069205D+02 2.080947143D+00 2.639078305D-03-2.714101362D-06
 1.402864982D-09-9.724321640D-14               -1.737850969D+03-8.133166800D+00
Cu(L)             Liquid. Ref-Elm.Cox,1989 p226.
 1 coda89 CU  1.00    0.00    0.00    0.00    0.00 2     63.54600          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 3.944910764D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -2.111013775D+02-1.836065775D+01
D2                Ref-Species. Gurvich,1989 v1 pt1 p134 pt2 p45.
 3 tpis89 D   2.00    0.00    0.00    0.00    0.00 0    4.0282040          0.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8569.103
 2.125790482D+04-2.996945907D+02 5.130314980D+00-4.172970890D-03 5.014345720D-06
-2.126389969D-09 2.386536969D-13 0.000000000D+00 3.944985900D+02-1.164191209D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8569.103
 8.215168560D+05-2.365623159D+03 5.342974510D+00 6.928145990D-05-8.523671020D-08
 2.456447415D-11-1.960597698D-15 0.000000000D+00 1.434214587D+04-1.712600356D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8569.103
 4.899848740D+08-3.112892916D+05 7.945961340D+01-8.425828740D-03 4.789458020D-07
-1.390917969D-11 1.637606941D-16 0.000000000D+00 2.460108052D+06-6.637009520D+02
e-                Ref-Species. Chase,1998 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
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F2                Ref-Elm. Gurvich,1989. v1 pt1 p157 pt2 p73.
 2 tpis89 F   2.00    0.00    0.00    0.00    0.00 0     37.99681          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
Fe(a)             Alpha. Ref-Elm.Below Lambda trans. Chase,1998 p1221.
 3 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 1     55.84500          0.000
    200.000    500.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4507.000
 1.350490931D+04-7.803806250D+02 9.440171470D+00-2.521767704D-02 5.350170510D-05
-5.099094730D-08 1.993862728D-11                2.416521408D+03-4.749002850D+01
    500.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4507.000
 3.543032740D+06-2.447150531D+04 6.561020930D+01-7.043929680D-02 3.181052870D-05
 0.000000000D+00 0.000000000D+00                1.345059978D+05-4.133788690D+02
    800.000   1042.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4507.000
 2.661026334D+09-7.846827970D+06-7.289212280D+02 2.613888297D+01-3.494742140D-02
 1.763752622D-05-2.907723254D-09                5.234868470D+07-1.529052200D+04
Fe(a)             Alpha. Ref-Elm.Above Lambda trans. Chase,1998 p1221.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 2     55.84500          0.000
   1042.000   1184.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4507.000
 2.481923052D+08 0.000000000D+00-5.594349090D+02 3.271704940D-01 0.000000000D+00
 0.000000000D+00 0.000000000D+00                6.467503430D+05 3.669168720D+03
Fe(c)             Gamma. Ref-Elm. Chase,1998 p1221.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 3     55.84500          0.000
   1184.000   1665.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4507.000
 1.442428576D+09-5.335491340D+06 8.052828000D+03-6.303089630D+00 2.677273007D-03
-5.750045530D-07 4.718611960D-11                3.264264250D+07-5.508852170D+04
Fe(d)             Delta. Ref-Elm. Chase,1998 p1221.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 4     55.84500          0.000
   1665.000   1809.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4507.000
-3.450190030D+08 0.000000000D+00 7.057501520D+02-5.442977890D-01 1.190040139D-04
 0.000000000D+00 0.000000000D+00                -8.045725750D+05-4.545180320D+03
Fe(L)             Liquid. Ref-Elm. Chase,1998 p1221.
 1 j 3/78 FE  1.00    0.00    0.00    0.00    0.00 5     55.84500          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 5.535383324D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.270608703D+03-2.948115042D+01
Ga(cr)            Rhombic. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.
 1 tpis96 GA  1.00    0.00    0.00    0.00    0.00 1     69.72300          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)             Liquid. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.
 1 tpis96 GA  1.00    0.00    0.00    0.00    0.00 2     69.72300          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
Ge(cr)             Cubic. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.
 2 tpis91 GE  1.00    0.00    0.00    0.00    0.00 1     72.61000          0.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4636.360
-2.396506145D+05 3.150572150D+03-1.333941357D+01 3.647997810D-02-2.942104614D-05
 0.000000000D+00 0.000000000D+00                -1.613882957D+04 7.939211600D+01
    400.000   1211.4007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4636.360
-1.888241797D+04 0.000000000D+00 2.898173070D+00 3.591659130D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.433864080D+02-1.298669726D+01
Ge(L)              Liquid. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.
 1 tpis91 GE  1.00    0.00    0.00    0.00    0.00 2     72.61000          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 3.319498082D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                3.278996640D+03-1.185992953D+01
H2                 Ref-Elm. Gurvich,1978 v1 pt2 1978 p31.
 3 tpis78 H   2.00    0.00    0.00    0.00    0.00 0      2.01588          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8468.102
 4.078323210D+04-8.009186040D+02 8.214702010D+00-1.269714457D-02 1.753605076D-05
-1.202860270D-08 3.368093490D-12                2.682484665D+03-3.043788844D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8468.102
 5.608128010D+05-8.371504740D+02 2.975364532D+00 1.252249124D-03-3.740716190D-07
 5.936625200D-11-3.606994100D-15                5.339824410D+03-2.202774769D+00
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8468.102
 4.966884120D+08-3.147547149D+05 7.984121880D+01-8.414789210D-03 4.753248350D-07
-1.371873492D-11 1.605461756D-16                2.488433516D+06-6.695728110D+02
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He                Ref-Elm. Moore,1971; Moore,1970a.
 3 g 5/97 HE  1.00    0.00    0.00    0.00    0.00 0      4.00260          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
Hg(cr)            Tetragonal. Ref-Elm. Chase,1998 p1373.
 1 j12/61 HG  1.00    0.00    0.00    0.00    0.00 1    200.59000          0.000
    100.000    234.2907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9343.000
-3.184586610D+03 0.000000000D+00 3.464424870D+00-4.054864610D-03 1.766281131D-05
 0.000000000D+00 0.000000000D+00               -1.282454336D+03-1.132010161D+01
Hg(L)             Liquid. Ref-Elm. Chase,1998 p1373.
 2 j12/61 HG  1.00    0.00    0.00    0.00    0.00 2    200.59000          0.000
    234.290    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9343.000
 1.058325418D+05-1.993826150D+03 1.880577074D+01-5.994680920D-02 1.228327030D-04
-1.293155349D-07 5.530734430D-11                7.916778390D+03-9.064871100D+01
    600.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         9343.000
 7.913840080D+05-3.956327060D+03 1.106465862D+01-8.153982650D-03 4.970504160D-06
-1.510428227D-09 1.872051162D-13                2.213772421D+04-6.072461670D+01
I2(cr)            Rhombic. Ref-Elm. Gurvich,1989 pt1 p219 pt2 p315.
 1 tpis89 I   2.00    0.00    0.00    0.00    0.00 1    253.80894          0.000
    200.000    386.7507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        13196.000
-3.901269140D+06 9.143202330D+04-8.900457500D+02 4.671270160D+00-1.357161837D-02
 2.073947355D-05-1.292905191D-08               -3.912632630D+05 4.422603650D+03
I2(L)             Liquid. Ref-Elm. Gurvich,1989 pt1 p219 pt2 p315.
 1 tpis89 I   2.00    0.00    0.00    0.00    0.00 2    253.80894          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 9.568212679D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.204453805D+03-3.637326088D+01
In(cr)            Tetragonal. Ref-Elm. Gurvich,1996 v3 pt1 255 pt2 p207.
 1 tpis96 IN  1.00    0.00    0.00    0.00    0.00 1    114.81800          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
In(L)             Liquid. Ref-Elm. Gurvich,1996 v3 pt1 255 pt2 p207.
 1 tpis96 IN  1.00    0.00    0.00    0.00    0.00 2    114.81800          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
K(cr)             Cubic. Ref-Elm. Cox,1989.
 1 coda89 K   1.00    0.00    0.00    0.00    0.00 1     39.09830          0.000
    200.000    336.8607 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7088.000
-1.022031747D+05 0.000000000D+00 1.333752016D+01-5.580990750D-02 9.013009100D-05
 0.000000000D+00 0.000000000D+00               -2.635062430D+03-5.615376520D+01
K(L)              Liquid. Ref-Elm. Cox,1989.
 1 coda89 K   1.00    0.00    0.00    0.00    0.00 2     39.09830          0.000
    336.860   2200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7088.000
-3.935722030D+03-4.547278110D+01 4.845244000D+00-3.083546588D-03 2.015548866D-06
-3.706172930D-11 5.032895480D-15               -8.075609680D+02-1.836641748D+01
Kr                Ref-Elm. Sugar,1991.
 3 g 8/97 KR  1.00    0.00    0.00    0.00    0.00 0     83.80000          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
Li(cr)            Crystal. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.
 2 tpis82 LI  1.00    0.00    0.00    0.00    0.00 1      6.94100          0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4632.000
-9.860652350D+03 0.000000000D+00 2.304323850D+00 2.671663720D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -8.388536120D+02-1.047881686D+01
    298.150    453.6907 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4632.000
 7.238824960D+04 0.000000000D+00 1.570314469D-01 6.770404110D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.049497436D+02 9.961763140D-01
Li(L)             Liquid. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.
 1 tpis82 LI  1.00    0.00    0.00    0.00    0.00 2      6.94100          0.000
    453.690   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4632.000
 2.465569228D+04 0.000000000D+00 3.755723428D+00-6.332303407D-04 3.160739478D-07
 0.000000000D+00 0.000000000D+00               -7.299116690D+02-1.701274654D+01
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Mg(cr)            Hexagonal. Ref-Elm. Alcock,1993.
 2 srd 93 MG  1.00    0.00    0.00    0.00    0.00 1     24.30500          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. Ref-Elm.  Alcock,1993.
 1 srd 93 MG  1.00    0.00    0.00    0.00    0.00 2     24.30500          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
Mn(a)             Alpha. Ref-Elm. Chase,1998 p1571.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 1     54.93805          0.000
    200.000    980.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4994.000
-1.984724642D+04 1.808814126D+02 1.038289801D+00 8.813332010D-03-1.298045968D-05
 1.118858744D-08-3.673641300D-12                -1.704143022D+03-3.713160980D+00
Mn(b)             Beta. Ref-Elm. Chase,1998 p1571.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 2     54.93805          0.000
    980.000   1361.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4994.000
-2.033299729D+08 8.595009270D+05-1.444429639D+03 1.217025958D+00-5.092264580D-04
 8.499457640D-08 0.000000000D+00                -5.153128480D+06 9.753553620D+03
Mn(c)             Gamma. Ref-Elm. Chase,1998 p1571.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 3     54.93805          0.000
   1361.000   1412.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4994.000
-5.539443490D+06 0.000000000D+00 1.249195042D+01-3.172888290D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.319440868D+04-7.701110710D+01
Mn(d)             Delta. Ref-Elm. Chase,1998 p1571.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 4     54.93805          0.000
   1412.000   1519.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4994.000
-4.256613510D+06 0.000000000D+00 1.001289188D+01-1.726727732D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.000110470D+04-6.059129950D+01
Mn(L)             Liquid. Ref-Elm. Chase,1998 p1571.
 1 j 9/67 MN  1.00    0.00    0.00    0.00    0.00 5     54.93805          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 5.535383324D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -9.393783130D+02-2.853570386D+01
Mo(cr)            Crystal. Ref-Elm. Chase,1998 p1577.
 3 j 3/78 MO  1.00    0.00    0.00    0.00    0.00 1     95.94000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4585.000
-4.961689320D+04 4.280941190D+02 7.671984690D-01 5.731518250D-03-6.381641180D-06
 3.708192420D-09-7.917347080D-13                -3.039584622D+03-1.230467690D+00
   1000.000   2200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4585.000
-3.617592720D+06 1.474639904D+04-2.136672658D+01 2.118577261D-02-9.789741690D-06
 2.496130112D-09-2.422303123D-13                -8.977896080D+04 1.507160275D+02
   2200.000   2896.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4585.000
 4.759909590D+09-5.321527320D+06-8.747403120D+02 3.794789480D+00-2.131568725D-03
 4.974075900D-07-4.325425090D-11                 4.096569650D+07 1.130483988D+02
Mo(L)             Liquid. Ref-Elm. Chase,1998 p1577.
 1 j 3/78 MO  1.00    0.00    0.00    0.00    0.00 2     95.94000          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 4.528949992D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 2.022300696D+03-2.280790783D+01
N2                Ref-Elm. Gurvich,1978 pt1 p280 pt2 p207.
 3 tpis78 N   2.00    0.00    0.00    0.00    0.00 0     28.01348          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
Na(cr)            Cubic. Ref-Elm. Cox,1989 p254.
 1 coda89 NA  1.00    0.00    0.00    0.00    0.00 1     22.98977          0.000
    200.000    371.0107 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6460.000
-3.584458010D+04 0.000000000D+00 6.479414690D+00-1.898697341D-02 3.352387090D-05
 0.000000000D+00 0.000000000D+00                -1.504319740D+03-2.677783039D+01
Na(L)             Liquid. Ref-Elm. Cox,1989 p254.
 1 coda89 NA  1.00    0.00    0.00    0.00    0.00 2     22.98977          0.000
    371.010   2300.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6460.000
 2.694818670D+04-2.319000780D+02 5.162435690D+00-3.058571990D-03 1.696407999D-06
-1.519633426D-10 1.962859159D-14                 2.842114288D+02-2.225763980D+01
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Nb(cr)            Crystal. Ref-Elm. Chase,1998 p1675.
 3 j12/73 NB  1.00    0.00    0.00    0.00    0.00 1     92.90638          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
-4.254811710D+04 3.875297090D+02 1.184449739D+00 4.507436620D-03-5.232091980D-06
 3.513452460D-09-9.507605800D-13               -2.864449323D+03-2.442975114D+00
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
 2.527695630D+07-1.085720528D+05 1.929168202D+02-1.727427651D-01 8.671274570D-05
-2.266162374D-08 2.437387316D-12                6.472317770D+05-1.284027328D+03
   2000.000   2750.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5241.000
 9.016788690D+08-1.888649522D+06 1.578845370D+03-6.588882220D-01 1.416307803D-04
-1.396561356D-08 4.411624050D-13                1.264760547D+07-1.175157316D+04
Nb(L)             Liquid. Ref-Elm. Chase,1998 p1675.
 1 j12/73 NB  1.00    0.00    0.00    0.00    0.00 2     92.90638          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 4.025733326D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                1.427029683D+03-1.857965621D+01
Ne                Ref-Elm. Moore,1971. Moore,1970a.
 3 g 5/97 NE  1.00    0.00    0.00    0.00    0.00 0     20.17970          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
 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
Ni(cr)            Crystal Ref-Elm. <lambda trans 631K. Chase,1998 p1697.
 2 j12/76 NI  1.00    0.00    0.00    0.00    0.00 1     58.69340          0.000
    200.000    400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4786.000
-7.689131090D+05 1.433956218D+04-1.042751331D+02 3.926261320D-01-6.986906890D-04
 4.906078910D-07 0.000000000D+00               -6.543789970D+04 5.511391170D+02
    400.000    631.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4786.000
-3.345887340D+08 3.424527970D+06-1.394425564D+04 2.825654843D+01-2.847789131D-02
 1.142789828D-05 0.000000000D+00               -1.750250768D+07 8.179861400D+04
Ni(cr)            Crystal Ref-Elm. >lambda trans 631K. Chase,1998 p1697.
 2 j12/76 NI  1.00    0.00    0.00    0.00    0.00 2     58.69340          0.000
    631.000   1200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4786.000
 1.036354737D+09-6.813278550D+06 1.854367615D+04-2.673006535D+01 2.153531609D-02
-9.192464140D-06 1.624332987D-09                3.771960950D+07-1.157617522D+05
   1200.000   1728.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4786.000
 2.518440662D+09-9.895465230D+06 1.609737530D+04-1.386478566D+01 6.671320910D-03
-1.698988160D-06 1.788537986D-10                5.987658740D+07-1.087743318D+05
Ni(L)             Liquid. Ref-Elm. Chase,1998 p1697.
 1 j12/76 NI  1.00    0.00    0.00    0.00    0.00 3     58.69340          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 4.679890938D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -3.216258550D+02-2.335474714D+01
O2                Ref-Elm. Gurvich,1989 pt1 p94 pt2 p9.
 3 tpis89 O   2.00    0.00    0.00    0.00    0.00 0    31.9988000          0.000
    200.000  1000.000 7 -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 0.000000000D+00-3.391454870D+03 1.849699470D+01
   1000.000  6000.000 7 -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 0.000000000D+00-1.689010929D+04 1.738716506D+01
   6000.000 20000.000 7 -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 0.000000000D+00 2.293554027D+06-5.530621610D+02
P(cr)             White. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326.
 1 tpis89 P   1.00    0.00    0.00    0.00    0.00 1     30.97376          0.000
    195.400    317.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5360.000
-4.761561170D+06 1.135422659D+05-1.120481079D+03 5.889005080D+00-1.727002916D-02
 2.689248597D-05-1.737186959D-08               -4.829321490D+05 5.551556600D+03
P(L)              Liquid. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326.
 1 tpis89 P   1.00    0.00    0.00    0.00    0.00 2     30.97376          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 3.141496011D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -8.621436240D+02-1.272272999D+01
Pb(cr)            Cubic. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.
 1 tpis91 PB  1.00    0.00    0.00    0.00    0.00 1    207.20000          0.000
    200.000    600.6507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6870.000
-6.149670140D+05 1.065718060D+04-7.129898940D+01 2.668406702D-01-5.182017320D-04
 5.238665090D-07-2.151645616D-10               -4.974077560D+04 3.855826030D+02
Pb(L)             Liquid. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.
 1 tpis91 PB  1.00    0.00    0.00    0.00    0.00 2    207.20000          0.000
    600.650   3600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6870.000
-3.798179327D+04 0.000000000D+00 4.364298076D+00-1.236392764D-03 4.946773773D-07
-5.231817630D-11 0.000000000D+00               -8.887330420D+02-1.619559677D+01
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Rb(cr)            Cubic. Ref-Elm. Cox,1989. Chase,1998 p1849 12/83.
 1 coda89 RB  1.00    0.00    0.00    0.00    0.00 1     85.46780          0.000
    100.000    312.4707 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7489.000
-1.693678854D+05 5.116764690D+03-5.686760910D+01 3.403543550D-01-9.347996350D-04
 1.017512352D-06 0.000000000D+00                -2.164547399D+04 2.805351095D+02
Rb(L)             Liquid. Ref-Elm. Cox,1989.
 2 coda89 RB  1.00    0.00    0.00    0.00    0.00 2     85.46780          0.000
    312.470   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7489.000
 2.365752770D+04 2.865695009D+02 1.546589030D+00 5.164698120D-03-6.065846790D-06
 3.347806150D-09-5.178101420D-13                -1.933656171D+03 1.060307276D+00
   1000.000   2100.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         7489.000
-3.672685780D+05 1.779065421D+03-3.414096790D-01 5.322070690D-03-4.262302730D-06
 1.699676170D-09-4.416789770D-14                -1.110894373D+04 1.477099469D+01
Rn                Ref-Elm. Moore,1971.
 3 g 5/97 RN  1.00    0.00    0.00    0.00    0.00 0    222.01760          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
S(a)              Alpha. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
 1 tpis89 S   1.00    0.00    0.00    0.00    0.00 1     32.06600          0.000
    200.000    368.3007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
-1.035710779D+04 0.000000000D+00 1.866766938D+00 4.256140250D-03-3.265252270D-06
 0.000000000D+00 0.000000000D+00                -7.516389580D+02-7.961066980D+00
S(b)              Beta. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
 1 tpis89 S   1.00    0.00    0.00    0.00    0.00 2     32.06600          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 2.080514131D+00 2.440879557D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -6.852714730D+02-8.607846750D+00
S(L)              Liquid. Ref-Elm. Gurvich,1989 pt1 p265 pt2 p160.
 5 tpis89 S   1.00    0.00    0.00    0.00    0.00 3     32.06600          0.000
    388.360    428.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
-6.366550765D+07 0.000000000D+00 2.376860693D+03-7.888076026D+00 7.376076522D-03
 0.000000000D+00 0.000000000D+00                -6.356594920D+05-1.186929589D+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 6.928522306D+03-3.254655981D+01 3.824448176D-02
 0.000000000D+00 0.000000000D+00                -9.832222680D+05-3.154806751D+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 1.649945697D+02-6.843534977D-01 7.315907973D-04
 0.000000000D+00 0.000000000D+00                -2.638846929D+04-7.681730097D+02
    453.150    717.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4412.000
 1.972984578D+06 0.000000000D+00-2.441009753D+01 6.090352889D-02-3.744069103D-05
 0.000000000D+00 0.000000000D+00                 1.113013440D+04 1.363174183D+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 3.848693429D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -8.284589830D+02-1.736128237D+01
Sc(a)             Alpha.  Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.
 2 tpis82 SC  1.00    0.00    0.00    0.00    0.00 1     44.95591          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.  Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.
 1 tpis82 SC  1.00    0.00    0.00    0.00    0.00 2     44.95591          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.  Ref-Elm. Gurvich,1982 pt1 p137 pt2 p138.
 1 tpis82 SC  1.00    0.00    0.00    0.00    0.00 3     44.95591          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)            Cubic. Ref-Elm. Gurvich,1991 pt1 p236 pt2 p220.
 2 tpis91 SI  1.00    0.00    0.00    0.00    0.00 1     28.08550          0.000
    200.000    298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         3217.471
-2.323538208D+04 0.000000000D+00 2.102021680D+00 1.809220552D-03 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.850635210D+02-1.038427318D+01
    298.150   1690.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         3217.471
-5.232559740D+04 0.000000000D+00 2.850169415D+00 3.975166970D-04 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.042947234D+03-1.438964187D+01
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Si(L)             Liquid. Ref-Elm. Gurvich,1991 pt1 p236 pt2 p220.
 1 tpis91 SI  1.00    0.00    0.00    0.00    0.00 2     28.08550          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 3.271389414D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                 4.882667110D+03-1.326611073D+01
Sn(cr)            CrI,tetragonal. Ref-Elm. Gurvich,1991 pt1 p350 pt2 p300.
 1 tpis91 SN  1.00    0.00    0.00    0.00    0.00 1    118.71000          0.000
    200.000    505.1187 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6323.000
-9.970568110D+05 1.865056292D+04-1.393005103D+02 5.652800870D-01-1.229162587D-03
 1.398259924D-06-6.465843270D-10                -8.479846440D+04 7.317981190D+02
Sn(L)             Liquid. Ref-Elm. Gurvich,1991 pt1 p350 pt2 p300.
 1 tpis91 SN  1.00    0.00    0.00    0.00    0.00 2    118.71000          0.000
    505.118   4700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6323.000
 9.847844311D+04 0.000000000D+00 3.028921728D+00 2.531718646D-04-1.960428215D-08
 0.000000000D+00 0.000000000D+00                 2.209652103D+02-9.089783541D+00
Sr(a)             Alpha. Ref-Elm. Alcock,1993.
 2 srd 93 SR  1.00    0.00    0.00    0.00    0.00 1     87.62000          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. Ref-Elm. Alcock,1993.
 1 srd 93 SR  1.00    0.00    0.00    0.00    0.00 2     87.62000          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. Ref-Elm. Alcock,1993.
 1 srd 93 SR  1.00    0.00    0.00    0.00    0.00 3     87.62000          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
Ta(cr)            Crystal. Ref-Elm. Chase,1998 p1899.
 3 j12/72 TA  1.00    0.00    0.00    0.00    0.00 1    180.94790          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
 1.519941999D+04-4.927143830D+02 6.855605760D+00-1.366625579D-02 2.561466303D-05
-2.235631116D-08 7.389831320D-12                 1.236077891D+03-3.252075490D+01
   1000.000   2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
-1.002219854D+08 4.696591430D+05-8.992639340D+02 9.084714280D-01-5.043323480D-04
 1.463919859D-07-1.734426993D-11                -2.762235634D+06 5.939534460D+03
   2000.000   3258.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5681.000
 3.305034810D+05 8.564351680D+01-1.797593491D+00 6.549784340D-03-2.878793550D-06
 4.952725110D-10-7.703452530D-15                 1.556933077D+03 1.641047132D+01
Ta(L)             Liquid. Ref-Elm. Chase,1998 p1899.
 1 j12/72 TA  1.00    0.00    0.00    0.00    0.00 2    180.94790          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 5.032166658D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -7.436042760D+02-2.597362534D+01
Th(a)             Alpha. Ref-Elm. Cox,1989 p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 1    232.03810          0.000
    200.000   1650.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6350.000
-1.453247151D+04 1.505222433D+02 2.270694767D+00 2.058614354D-03-9.216614670D-07
 4.316796340D-10-7.950656800D-14                -1.667536353D+03-6.857176980D+00
Th(b)             Beta. Ref-Elm. Cox,1989 p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 2    232.03810          0.000
   1650.000   2023.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6350.000
 8.360316570D+06-2.333327743D+04 2.783594798D+01-1.293559561D-02 3.966098040D-06
-4.361984440D-10 0.000000000D+00                 1.501326293D+05-1.894583434D+02
Th(L)             Liquid. Ref-Elm. Cox,1989 p239.
 1 coda89 TH  1.00    0.00    0.00    0.00    0.00 3    232.03810          0.000
   2023.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6350.000
 0.000000000D+00 0.000000000D+00 5.532496804D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.191824935D+03-2.760071917D+01
Ti(a)             Alpha Crystal. Ref-Elm. Cox,1989 p230.
 2 coda89 TI  1.00    0.00    0.00    0.00    0.00 1     47.86700          0.000
    200.000    900.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4824.000
 3.598601350D+04-8.272305960D+02 7.689097770D+00-1.143968449D-02 1.392105464D-05
-4.691057160D-09-9.852130400D-13                 2.936621421D+03-3.985138010D+01
    900.000   1156.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4824.000
-2.876235910D+06 0.000000000D+00 4.573153420D+01-7.692381600D-02 3.799919490D-05
 0.000000000D+00 0.000000000D+00                -2.038023972D+04-2.516270281D+02
Ti(b)             Beta Crystal. Ref-Elm. Cox,1989 p230.
 1 coda89 TI  1.00    0.00    0.00    0.00    0.00 2     47.86700          0.000
   1156.000   1944.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4824.000
-1.698740574D+06 6.576601240D+03-8.556182950D+00 9.789585830D-03-3.992418760D-06
 1.123642773D-09-1.201048055D-13                -3.929918290D+04 6.506590190D+01
```

```
Ti(L)             Liquid. Ref-Elm. Cox,1989 p230.
 1 coda89 TI  1.00    0.00    0.00    0.00    0.00 3     47.86700          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 5.628714139D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.377354619D+03-3.079443471D+01
U(a)              Alpha. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 1    238.02890          0.000
    200.000    942.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6364.000
-1.540899462D+04 2.318801962D+02 1.227944510D+00 7.136117480D-03-1.018038579D-05
 1.136884370D-08-3.669367430D-12                -1.986921870D+03-2.035974193D+00
U(b)              Beta. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 2    238.02890          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 5.099518793D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.672080149D+03-2.378030116D+01
U(c)              Gamma. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 3    238.02890          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 4.606404947D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -5.859187270D+02-1.980809042D+01
U(L)              Liquid. Ref-Elm. Cox,1989 p234.
 1 coda89 U   1.00    0.00    0.00    0.00    0.00 4    238.02890          0.000
   1408.000   4000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         6364.000
-9.466562120D+04 8.526619680D+02 4.209128020D+00 8.407200810D-04-1.309545676D-07
 1.985020032D-11-1.231574075D-15                -5.956398090D+03-1.667247672D+01
V(cr)             Crystal. Ref-Elm. Chase,1998 p1917.
 3 j 6/73 V   1.00    0.00    0.00    0.00    0.00 1     50.94150          0.000
    200.000    600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 2.845125913D+05-5.094932860D+03 3.715018720D+01-1.176030941D-01 2.255823526D-04
-2.260642686D-07 9.289596800D-11                2.254378204D+04-1.968241679D+02
    600.000   1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 1.372056465D+06-7.847553620D+03 2.095142247D+01-2.055640932D-02 1.323266530D-05
-4.042182900D-09 5.087521100D-13                4.374800000D+04-1.292763446D+02
   1400.000   2190.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4640.000
 5.281067680D+08-1.907420191D+06 2.862656637D+03-2.277492896D+00 1.017078880D-03
-2.412149691D-07 2.377114537D-11                1.169890783D+07-1.956716732D+04
V(L)              Liquid. Ref-Elm. Chase,1998 p1917.
 1 j 6/73 V   1.00    0.00    0.00    0.00    0.00 2     50.94150          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 5.557032224D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -1.899700630D+03-3.070532450D+01
W(cr)             Crystal. Ref-Elm. Chase,1998 p1925.
 4 j 6/66 W   1.00    0.00    0.00    0.00    0.00 1    183.84000          0.000
    200.000   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4973.000
-6.824541400D+03-2.254249090D+02 4.976604610D+00-6.926436340D-03 1.202272986D-05
-9.344133510D-09 2.818887123D-12                -3.510679270D+00-2.361334984D+01
   1000.000   2600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4973.000
 5.530134840D+05-2.041485344D+03 5.870839470D+00-1.920714198D-03 1.067652983D-06
-2.355109022D-10 2.160679310D-14                1.163812518D+04-3.319171800D+01
   2600.000   3200.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4973.000
 2.474736879D+09 4.488921620D+06-1.235978300D+04 9.678565660D+00-3.556364610D-03
 6.380420610D-07-4.521123450D-11                -2.029500909D+07 8.274369690D+04
   3200.000   3680.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         4973.000
-1.755550399D+10 1.179059156D+07 1.177715365D+03-2.675166841D+00 7.252172480D-04
-6.128007580D-08 0.000000000D+00                -9.702249190D+07-1.148926234D+03
W(L)              Liquid. Ref-Elm. Chase,1998 p1925.
 1 j 6/66 W   1.00    0.00    0.00    0.00    0.00 2    183.84000          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 4.277341659D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                2.755443078D+03-2.086449853D+01
Xe                Ref-Elm. Moore,1971. Moore,1971a.
 3 g 1/99 XE  1.00    0.00    0.00    0.00    0.00 0    131.29000          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
```

```
Zn(cr)            Crystal. Ref-Elm. Cox,1989 p221.
 1 coda89 ZN  1.00    0.00    0.00    0.00    0.00 1     65.39000          0.000
    200.000    692.7307 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5657.000
 3.702080380D+05-5.915475500D+03 3.959500360D+01-1.143735885D-01 1.934363797D-04
-1.675385126D-07 6.078189940D-11                2.681737238D+04-2.114848186D+02
Zn(L)             Liquid. Ref-Elm. Cox,1989 p221.
 1 coda89 ZN  1.00    0.00    0.00    0.00    0.00 2     65.39000          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 3.776530427D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -4.317345880D+02-1.567077937D+01
Zr(a)             Alpha. Ref-Elm. Chase,1998 p1943.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 1     91.22400          0.000
    200.000   1135.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5497.000
-1.153699220D+04 2.626203401D+01 2.932054698D+00 5.743358570D-04-7.651710410D-07
 1.597202829D-09-6.097129620D-13               -1.084153260D+03-1.215776960D+01
Zr(b)             Beta. Ref-Elm. Chase,1998 p1943.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 2     91.22400          0.000
   1135.000   2125.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5497.000
-1.065463955D+06 4.273000010D+03-3.173856480D+00 5.018842560D-03-2.363431747D-06
 7.707582390D-10-8.156156570D-14               -2.641247444D+04 3.072041827D+01
Zr(L)             Liquid. Ref-Elm. Chase,1998 p1943.
 1 j 6/79 ZR  1.00    0.00    0.00    0.00    0.00 3     91.22400          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 5.032166658D+00 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00               -1.100795852D+03-2.548066000D+01
```

Appendix C
Required Format for Input Thermodynamic Coefficients

Equations (1) to (3) define the nine coefficients (a_1, $a_2 \ldots a_7$, b_1, and b_2) that describe the thermodynamic functions $C_p^o(T)/R$, $H^o(T)/RT$, and $S^o(T)/R$ for all species in the NASA Glenn database. As discussed in the text, separate thermodynamic coefficients are generated for each condensed phase. The CAP and CEA programs read in the thermodynamic coefficients in the format shown in table IC.

TABLE IC.—GENERAL FORMAT FOR NASA 9-CONSTANT COEFFICIENT RECORDS

Record	Contents	Fortran format	Columns
1	Species name or formula	A16	1 to 16
	Comments and data source	A62	19 to 80
2	Number of T intervals	I2	1 to 2
	Optional identification code	A6	4 to 9
	Chemical formula—symbols and numbers (all capitals)	5(A2, F6.2)	11 to 50
	Zero for gas, nonzero for condensed	I2	51 to 52
	Molecular weight	F13.7	53 to 65
	Heat of formation at 298.15 K, J/mol	F15.5	66 to 80
3	Temperature range	2F11.3	1 to 22
	Number of coefficients for $C_p^o(T)/R$	I1	23
	T exponents in empirical equation for $C_p^o(T)/R$	8F5.1	24 to 63
	$[H^o(298.15) - H^o(0)]$, J/mol	F15.3	66 to 80
4	First five coefficients for $C_p^o(T)/R$	5D16.9	1 to 80
5	Last two coefficients for $C_p^o(T)/R$	2D16.9	1 to 32
	Integration constants b_1 and b_2	2D16.9	49 to 80
--	Repeat 3, 4, and 5 for each interval	----	-----

The following data are for condensed titanium nitride:

```
    12345678901234567890123456789012345678901234567890123456789012345678901234567890
             10        20        30        40        50        60        70        80

1   TiN(cr)           JPCRD 1998 Mono.9 p1612-4.                                    1
2    2 j 6/68 TI  1.00N   1.00    0.00    0.00    0.00 1     61.87374    -337648.800    2
3       200.000    800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5487.000    3
4   -5.479117220D+05 9.328691110D+03-6.386263890D+01 2.429925456D-01-4.304234520D-04    4
5    3.792645100D-07-1.317412256D-10               -8.424256140D+04 3.392988560D+02    5
6       800.000   3220.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5487.000    6
7   -3.656247060D+05 1.265730431D+03 3.831711190D+00 1.632900455D-03-1.062786626D-07    7
8    1.310931390D-11-5.770548410D-16               -5.027654400D+04-1.652632899D+01    8
9   TiN(L)            JPCRD 1998 Mono.9 p1612-4.                                    9
10   1 j 6/68 TI  1.00N   1.00    0.00    0.00    0.00 2     61.87374    -337648.800    10
11     3220.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         5487.000    11
12   0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00    12
13   0.000000000D+00 0.000000000D+00               -3.626039860D+04-3.958296649D+01    13

    12345678901234567890123456789012345678901234567890123456789012345678901234567890
             10        20        30        40        50        60        70        80
```

There are two sets of data: one for the crystal and one for the liquid. Focusing first on the crystalline phase (records 1 to 8), record 1 lists the name as TiN(cr) and tells that the data for this phase originated from J. Phys. Chem. Ref. Data Monograph 9, 1998, pp. 161–214. Table IIC gives an explanation of Record 2, TiN data (See also table IC):

TABLE IIC.—EXPLANATION OF RECORD 2, TiN DATA

Columns	Contents	Explanation
1 to 2	2	Number of temperature intervals covered by the data
4 to 9	j 6/68	Internal NASA reference code (see appendix A)
11 to 19	TI1.0N1.0	Molecular formula unused places (20 to 50) filled with blanks and zeroes
51 to 52	1	(First) condensed phase
53 to 60	61.87374	Molecular weight (5 places unused)
66 to 74	–337648.8	$\Delta_f H^o$ (298.15) in J/mole (6 places unused)

Records 3 to 5 cover the temperature interval 200 to 800 K. The single digit "7" after the temperature range means that $C_p^o(T)/R$ is described by seven coefficients in each interval. This value can range from 1 to 8. The next eight 5-place fields on record 3 list the temperature exponents in the empirical equation for $C_p^o(T)/R$ used in this temperature interval. The last entry on record 3 contains a value of 5487.00 J/mole for $[H^o(298.15) - H^o(0)]$. This field will contain the number 0.0000 if $[H^o(298.15) - H^o(0)]$ is not available. Records 4 to 5 contain the coefficients a_1 through a_7, b_1, and b_2 for TiN(cr) for the temperature range 200 to 800 K; records 7 and 8 contain these coefficients for the temperature range 800 to 3220 K. Both intervals use equation (1) to describe $C_p^o(T)/R$.

Data for the liquid immediately follow the TiN(cr) data block. The temperature range 3220 K (melting point) to 6000 K is covered by one set of coefficients, again in the form of equation (1) with seven terms for $C_p^o(T)/R$. The zero values listed for all constants except a_3 indicate that, in accordance with equation (1), the heat capacity is a constant ($C_p^o/R = 7.548249987$).

Appendix D
CAP Input and Output Examples

Example 1 FO_2 listing 400 to 1000 K

This example illustrates (1) tabulated functions from NASA fitted coefficients, (2) format for input file, and (3) multiple keywords.

Example 1 input file:

```
     'mfig' 'logk' 'joules' /
     400,100,1000  /
FO2,FOO           Chase 1996 JPCRD v25 n2 p551.
 2 j 9/95 F   1.00O   2.00    0.00    0.00    0.00 0     50.99720      25400.000
    200.000   1000.0007 -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                2.694645218D+03-1.166414457D+00
   1000.000   6000.0007 -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               -1.596825164D+04 8.655417510D+00
```

Example 1 output from CAP:

```
 OPTIONS:  mfig    logk    joules


 TEMPERATURE SCHEDULE

    400.000     500.000     600.000     700.000     800.000     900.000
   1000.000


                                  ***** NOTE *****

  The temperature range of the coefficients read in the standard input (I/O unit 5)
  will be extended by 20 %.  E.g. a range of 300 to 5000 K will be extended to 240
  to 6000 K. The extrapolated data may have large errors. The element data cap.elms
  (I/O unit 13) will NOT be extrapolated when calculating delta H and log K.


                     COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS


    FO2,FOO           Chase 1996 JPCRD v25 n2 p551.
     2 j 9/95 F   1.00O   2.00    0.00    0.00    0.00 0     50.99720      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


  THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR FO2,FOO


    Assigned H(T) at    0.00 K =   14144.187 J/mol

      T          Cp          H-H0         S          -(G-H0)         H           -G
    deg-K      J/mol-K       J/mol      J/mol-K        J/mol        J/mol         J/mol

    400.00    47.42217    15942.683   273.012164    93262.183     30086.870     79117.996
    500.00    49.60339    20798.754   283.839126   121120.809     34942.941    106976.622
    600.00    51.29020    25846.991   293.038479   149976.096     39991.178    135831.909
    700.00    52.59593    31044.126   301.047311   179688.992     45188.313    165544.805
    800.00    53.59831    36356.071   308.138937   210155.079     50500.258    196010.892
    900.00    54.36861    41756.044   314.498300   241292.426     55900.231    227148.239
   1000.00    54.98396    47224.615   320.259446   273034.831     61368.802    258890.644
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR FO2,FOO

T deg-K	Cp J/mol-K	H-H298 kJ/mol	S J/mol-K	-(G-H298)/T J/mol-K	H kJ/mol	delta Hf kJ/mol	log K
0	0.	-11.256	0.	INFINITE	14.144	27.237	INFINITE
400	47.422	4.687	273.012	261.295	30.087	25.422	-5.7737
500	49.603	9.543	283.839	264.753	34.943	25.536	-5.1085
600	51.290	14.591	293.038	268.720	39.991	25.687	-4.6627
700	52.596	19.788	301.047	272.778	45.188	25.853	-4.3423
800	53.598	25.100	308.139	276.764	50.500	26.022	-4.1004
900	54.369	30.500	314.498	280.609	55.900	26.188	-3.9110
1000	54.984	35.969	320.259	284.291	61.369	26.349	-3.7586

This example illustrates the generation of thermodynamic functions for the FO_2 molecule in the standard many-figured (MFIG) format and in the log K format. Note the following important points:

1. The first two records in the input file end with a slash. These two records contain, respectively, the output keywords (page 3) and the temperature schedule (page 4).

2. Several output keywords may appear on the keyword record. Separate tables are printed for the output options specified.

3. The thermodynamic coefficients for this particular case were generated by the least-squares fit to data published in Chase (1996, p. 551). These fitted coefficients are used by CAP to generate the output tables. Thus, the output tables do not precisely match the tables published in the reference.

4. The MFIG tables contain the thermodynamic functions for enthalpy and Gibbs energy relative to 0 K. In contrast, for the LOGK tables, these functions are listed relative to 298.15 K.

5. The cap.elms file must be available and must contain the reference elements F_2 and O_2 in order for the program to generate $\Delta_f H^o(T)$ and log K values for FO_2. See page 4 and appendix B.

Example 2 $CaCl_2$ listing 200 to 1400 K in 200 K intervals

This example illustrates (1) the appearance of tables at a phase change, (2) nondefault energy units, and (3) gas-phase listings.

Example 2 input file: :

```
     'cal' 'nodim' 'logk' /
     200,200,1400  /
CaCL2(cr)         Rhombic. TPIS 1996 pt1 p467 pt2 p365.
 2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 1    110.98340    -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    110.98340    -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
CaCL2             Hsubl & cons: TPIS v3 pt1 p470 pt2 p366.
 2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 0    110.98340    -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
```

Example 2 output from CAP:

```
KEYWORDS:  cal    nodi   logk


TEMPERATURE SCHEDULE

   200.000     298.150     400.000     600.000     800.000    1000.000
  1200.000    1400.000


                                ***** NOTE *****

 The temperature range of the coefficients read in the standard input (I/O unit 5)
 will be extended by 20 %.  E.g. a range of 300 to 5000 K will be extended to 240
 to 6000 K. The extrapolated data may have large errors. The element data cap.elms
 (I/O unit 13) will NOT be extrapolated when calculating delta H and log K.


                    COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS


    CaCL2(cr)         Rhombic. TPIS 1996 pt1 p467 pt2 p365.
     2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 1    110.98340    -795800.000
        100.000   500.000 7 -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 0.000000000D+00-9.606057780D+04-3.912159570D+01
        500.000  1048.000 7 -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 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    110.98340    -795800.000
       1048.000  6000.000 7 -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 0.000000000D+00-9.391818610D+04-4.566953897D+01
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CaCL2(cr) CaCL2(L)

Assigned H(T)/R at 0.00 K = -97552.407 K

T	Cp/R	(H-H0)/RT	S/R	-(G-H0)/RT	H/RT	-G/RT
200.00	8.10040	5.0359305	9.6573322	4.6214017	-482.7261024	492.3834346
298.15	8.76131	6.1721008	13.0374490	6.8653482	-321.0202741	334.0577231
400.00	9.06625	6.8732504	15.6582746	8.7850242	-237.0077660	252.6660406
600.00	9.47875	7.6768753	19.4170689	11.7401936	-154.9104690	174.3275379
800.00	9.82139	8.1708288	22.1916169	14.0207880	-113.7696794	135.9612962
1000.00	10.14431	8.5334217	24.4180975	15.8846757	-89.0189848	113.4370823
1048.00	10.22044	8.6089479	24.8954714	16.2865235	-84.4754095	109.3708809
1048.00	13.20683	11.8280513	28.1145748	16.2865235	-81.2563061	109.3708809
1200.00	12.63182	11.9638168	29.8625860	17.8987692	-69.3298554	99.1924414
1400.00	12.14146	12.0215257	31.7700559	19.7485302	-57.6587647	89.4288206

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CaCL2(cr) CaCL2(L)

	T deg-K	Cp cal/mol-K	H-H298 kcal/mol	S cal/mol-K	-(G-H298)/T cal/mol-K	H kcal/mol	delta Hf kcal/mol	log K
	0	0.	-3.657	0.	INFINITE	-193.858	-190.281	INFINITE
	200	16.097	-1.655	19.191	27.468	-191.856	-190.494	199.6855
	298.15	17.411	0.000	25.908	25.908	-190.201	-190.201	131.2053
	400	18.017	1.807	31.116	26.600	-188.394	-189.881	95.7332
	600	18.836	5.496	38.586	29.425	-184.704	-189.288	61.1996
*	800	19.517	9.333	44.100	32.433	-180.868	-188.914	43.9791
	1000	20.159	13.301	48.524	35.223	-176.900	-188.216	33.6752
	1048	20.310	14.272	49.473	35.854	-175.929	-188.053	31.7921
	1048	26.245	20.976	55.870	35.854	-169.225	-181.349	31.7921
*	1200	25.102	24.873	59.343	38.616	-165.328	-182.179	26.9896
	1400	24.128	29.788	63.134	41.857	-160.413	-180.886	22.2663

*Assigned reference phase change at 716.00 K, 1115.00 K,

COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

```
CaCL2              Hsubl & cons: TPIS v3 pt1 p470 pt2 p366.
 2 tpis96 CA  1.00CL  2.00    0.00    0.00    0.00 0    110.98340    -485243.477
    200.000  1000.000 7 -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 0.000000000D+00-5.850346760D+04-1.808679105D+01
   1000.000  6000.000 7 -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 0.000000000D+00-6.066779660D+04-8.553531560D+00
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CaCL2

Assigned H(T)/R at 0.00 K = -60147.922 K

T	Cp/R	(H-H0)/RT	S/R	-(G-H0)/RT	H/RT	-G/RT
200.00	6.73649	5.5253550	31.6764550	26.1511000	-295.2142557	326.8907107
298.15	7.10204	5.9932213	34.4452652	28.4520439	-195.7438980	230.1891632
400.00	7.26570	6.2990305	36.5582501	30.2592197	-144.0707748	180.6290250
600.00	7.39121	6.6460637	39.5327242	32.8866604	-93.6004731	133.1331973
800.00	7.43803	6.8390152	41.6663918	34.8273766	-68.3458875	110.0122792
1000.00	7.46002	6.9612343	43.3287458	36.3675115	-53.1866878	96.5154336
1200.00	7.47211	7.0454633	44.6900360	37.6445727	-43.0778052	87.7678412
1400.00	7.47946	7.1069776	45.8424618	38.7354842	-35.8558239	81.6982857

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CaCL2

	T deg-K	Cp cal/mol-K	H-H298 kcal/mol	S cal/mol-K	-(G-H298)/T cal/mol-K	H kcal/mol	delta Hf kcal/mol	log K
	0	0.	-3.551	0.	INFINITE	-119.527	-115.950	INFINITE
	200	13.387	-1.355	62.948	69.722	-117.331	-115.969	127.8129
	298.15	14.113	0.000	68.450	68.450	-115.976	-115.976	86.0958
	400	14.439	1.456	72.649	69.009	-114.520	-116.007	64.4479
	600	14.688	4.373	78.560	71.271	-111.603	-116.186	43.3091
*	800	14.781	7.322	82.800	73.648	-108.654	-116.701	32.7096
	1000	14.825	10.283	86.104	75.821	-105.693	-117.010	26.3263
*	1200	14.849	13.250	88.809	77.767	-102.726	-119.576	22.0280
	1400	14.863	16.221	91.099	79.512	-99.755	-120.228	18.9089

*Assigned reference phase change at 716.00 K, 1115.00 K,

This example illustrates the format of output tables when phase changes occur. Note the following important points:

1. A table is printed for the NODIM and LOGK keywords. The NODIM table gives dimensionless data in many-figured format. The log K table uses cal/mole and kcal/mole.

2. A line is automatically inserted at 298.15 K in all tables.

3. A phase change occurs for $CaCl_2$ at 1048 K. An output line is printed for each phase.

4. Phase changes occur also in the reference element Ca at 716 K and at 1115 K. These are denoted by asterisks in the log K output tables at 800 K and 1200 K. A footnote at the end of the log K table lists all reference element phase changes encountered.

Example 3 O_2, S_2F_2, ScO^+, PO_2^- listing 200 to 10 000 K

This example illustrates (1) multiple chemical species, (2) log K special cases, and (3) temperature extrapolation of coefficient data.

Example 3 input file: :

```
     'logk' /
     200,100,1000,500,10000/
O2               TPIS 1989 v1 pt1 p94 pt2 p9.
 3 tpis89 O   2.00    0.00    0.00    0.00    0.00 0     31.99880          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
S2F2              Thiothionyl fluoride.JPCRD 1985 sup1 v14 pt2 p1105.
 2 j 6/76 S   2.00F   2.00    0.00    0.00    0.00 0    102.12881    -401413.000
    200.000   1000.0007 -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                -4.067208250D+04-4.560825680D+01
   1000.000   6000.0007 -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                -5.147675180D+04-2.375663203D+01
ScO+              D0,Estim.cons:TPIS 1982 v4 pt1 p142 pt2 p145.
 3 g10/99 SC  1.00O   1.00E  -1.00    0.00    0.00 0     60.95476     561209.966
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8777.066
 4.588560270D+04-3.367114370D+02 3.527206400D+00 3.988850300D-03-5.568985430D-06
 3.650281190D-09-9.356491500D-13                 6.838350790D+04 4.339812700D+00
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8777.066
-1.814357141D+06 5.853425320D+03-3.657101210D+00 5.734364510D-03-2.092878161D-06
 3.695645020D-10-2.214038347D-14                 2.955364078D+04 5.660889410D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8777.066
 4.395803280D+09-2.670232109D+06 6.250769670D+02-6.991767580D-02 4.175372710D-06
-1.274326266D-10 1.571603736D-15                 2.130530393D+07-5.428823800D+03
PO2-              TPIS 1989 v1 pt1 p409; pt2 p261.
 3 tpis89 P   1.00O   2.00E   1.00    0.00    0.00 0     62.97311    -597623.751
    298.150   1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 2.702423135D+04 2.939956284D+01 1.162686114D+00 1.599897972D-02-1.979229263D-05
 1.208847527D-08-2.956640480D-12                -7.285946270D+04 1.963118182D+01
   1000.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 1.628679152D+06-5.989199980D+03 1.369318836D+01-3.623843790D-03 9.488198340D-07
-1.040308759D-10 4.019033660D-15                -3.685959500D+04-5.956796220D+01
   6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 1.527048695D+08-1.152139645D+05 3.747485230D+01-3.443388910D-03 2.011144470D-07
-5.996871080D-12 7.244612160D-17                 8.207935510D+05-2.759665314D+02
```

Example 3 output from CAP:

```
OPTIONS:  logk


TEMPERATURE SCHEDULE

   200.000     298.150     300.000     400.000     500.000     600.000
   700.000     800.000     900.000    1000.000    1500.000    2000.000
  2500.000    3000.000    3500.000    4000.000    4500.000    5000.000
  5500.000    6000.000    6500.000    7000.000    7500.000    8000.000
  8500.000    9000.000    9500.000   10000.000

                                ***** NOTE *****

The temperature range of the coefficients read in the standard input (I/O unit 5)
will be extended by 20 %.  E.g. a range of 300 to 5000 K will be extended to 240
to 6000 K. The extrapolated data may have large errors. The element data cap.elms
(I/O unit 13) will NOT be extrapolated when calculating delta H and log K.




                    COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

   O2                TPIS 1989 v1 pt1 p94 pt2 p9.
    3 tpis89 O   2.00    0.00    0.00    0.00    0.00 0     31.99880          0.000
       200.000  1000.000 7 -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 0.000000000D+00-3.391454870D+03 1.849699470D+01
      1000.000  6000.000 7 -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 0.000000000D+00-1.689010929D+04 1.738716506D+01
      6000.000 20000.000 7 -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 0.000000000D+00 2.293554027D+06-5.530621610D+02



THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR O2

     T         Cp        H-H298        S      -(G-H298)/T      H        delta Hf     log K
   deg-K    J/mol-K      kJ/mol     J/mol-K     J/mol-K      kJ/mol      kJ/mol

     0        0.         -8.680       0.        INFINITE     -8.680        0       INFINITE
   200      29.126       -2.868     193.484     207.826      -2.868        0           0
   298.15   29.378        0.000     205.149     205.149       0.000        0           0
   300      29.388        0.054     205.331     205.150       0.054        0           0
   400      30.115        3.026     213.875     206.310       3.026        0           0
   500      31.092        6.086     220.698     208.527       6.086        0           0

   600      32.090        9.245     226.456     211.048       9.245        0           0
   700      32.990       12.500     231.472     213.615      12.500        0           0
   800      33.745       15.838     235.928     216.130      15.838        0           0
   900      34.361       19.244     239.939     218.557      19.244        0           0
  1000      34.883       22.707     243.587     220.880      22.707        0           0

  1500      36.553       40.613     258.086     231.010      40.613        0           0

  2000      37.784       59.202     268.772     239.171      59.202        0           0

  2500      38.933       78.384     277.328     245.975      78.384        0           0

  3000      39.980       98.117     284.521     251.815      98.117        0           0

  3500      40.904      118.344     290.755     256.942     118.344        0           0

  4000      41.707      139.001     296.271     261.520     139.001        0           0

  4500      42.400      160.032     301.224     265.661     160.032        0           0

  5000      42.997      181.385     305.723     269.446     181.385        0           0
```

5500	43.511	203.015	309.846	272.934	203.015	0	0
6000	43.950	224.884	313.651	276.170	224.884	0	0
6500	44.206	246.925	317.179	279.191	246.925	0	0
7000	44.338	269.069	320.461	282.023	269.069	0	0
7500	44.280	291.232	323.520	284.689	291.232	0	0
8000	44.023	313.315	326.370	287.206	313.315	0	0
8500	43.584	335.224	329.027	289.589	335.224	0	0
9000	42.992	356.874	331.502	291.849	356.874	0	0
9500	42.279	378.196	333.808	293.998	378.196	0	0
10000	41.477	399.138	335.956	296.042	399.138	0	0

COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

```
   S2F2              Thiothionyl fluoride.JPCRD 1985 sup1 v14 pt2 p1105.
    2 j 6/76 S   2.00F   2.00    0.00    0.00    0.00 0    102.12881    -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
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR S2F2

	T deg-K	Cp J/mol-K	H-H298 kJ/mol	S J/mol-K	-(G-H298)/T J/mol-K	H kJ/mol	delta Hf kJ/mol	log K
	0	0.	-13.718	0.	INFINITE	-415.131	-397.482	INFINITE
	200	52.613	-5.715	269.725	298.299	-407.128	-399.981	106.1204
	298.15	63.128	0.000	292.833	292.833	-401.413	-401.413	71.6770
	300	63.285	0.117	293.224	292.834	-401.296	-401.438	71.2433
*	400	69.879	6.803	312.413	295.405	-394.610	-407.179	53.7207
	500	73.872	14.007	328.471	300.457	-387.406	-411.211	43.0400
	600	76.370	21.528	342.177	306.297	-379.885	-414.325	35.8536
	700	78.002	29.252	354.081	312.292	-372.161	-416.846	30.6855
	800	79.122	37.112	364.574	318.184	-364.301	-419.004	26.7877
	900	79.925	45.066	373.942	323.868	-356.347	-421.105	23.7407
	1000	80.505	53.089	382.395	329.305	-348.324	-423.173	21.2909
	1500	81.942	93.770	415.365	352.851	-307.643	-433.331	13.8462
	2000	82.462	134.889	439.020	371.575	-266.524	-443.526	10.0338
	2500	82.707	176.188	457.450	386.975	-225.225	-453.726	7.6924
	3000	82.840	217.578	472.542	400.016	-183.835	-463.592	6.0961
	3500	82.921	259.020	485.318	411.313	-142.393	-472.795	4.9320
	4000	82.979	300.495	496.395	421.271	-100.918	-481.135	4.0425
	4500	83.028	341.997	506.171	430.172	-59.416	-488.555	3.3391
	5000	83.080	383.524	514.922	438.217	-17.889	-495.109	2.7683
	5500	83.144	425.079	522.843	445.556	23.666	-500.899	2.2953
	6000	83.228	466.671	530.081	452.302	65.258	-506.009	1.8969
	6500	83.343	508.312	536.747	458.545	106.899		
	7000	83.498	550.021	542.929	464.354	148.608		

*Assigned reference phase change at 388.36 K,

COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

```
ScO+              D0,Estim.cons:TPIS 1982 v4 pt1 p142 pt2 p145.
 3 g10/99 SC  1.00O   1.00E  -1.00    0.00    0.00 0     60.95476     561209.966
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8777.066
 4.588560270D+04-3.367114370D+02 3.527206400D+00 3.988850300D-03-5.568985430D-06
 3.650281190D-09-9.356491500D-13 0.000000000D+00 6.838350790D+04 4.339812700D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8777.066
-1.814357141D+06 5.853425320D+03-3.657101210D+00 5.734364510D-03-2.092878161D-06
 3.695645020D-10-2.214038347D-14 0.000000000D+00 2.955364078D+04 5.660889410D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8777.066
 4.395803280D+09-2.670232109D+06 6.250769670D+02-6.991767580D-02 4.175372710D-06
-1.274326266D-10 1.571603736D-15 0.000000000D+00 2.130530393D+07-5.428823800D+03
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR ScO+

	T deg-K	Cp J/mol-K	H-H298 kJ/mol	S J/mol-K	-(G-H298)/T J/mol-K	H kJ/mol	delta Hf kJ/mol	log K
	0	0.	-8.777	0.	INFINITE	552.433	555.783	INFINITE
	298.15	30.744	0.000	218.504	218.504	561.210	561.210	-92.9842
	300	30.773	0.057	218.694	218.504	561.267	561.231	-92.3779
	400	32.313	3.212	227.761	219.730	564.422	562.382	-67.9262
	500	33.568	6.509	235.113	222.094	567.719	563.567	-53.2244
	600	34.498	9.915	241.320	224.795	571.125	564.754	-43.4023
	700	35.176	13.401	246.692	227.548	574.611	565.908	-36.3719
	800	35.675	16.944	251.423	230.242	578.154	566.998	-31.0886
	900	36.052	20.532	255.647	232.835	581.742	568.004	-26.9716
	1000	36.342	24.152	259.461	235.310	585.362	568.908	-23.6725
	1500	37.137	42.554	274.374	246.004	603.764	571.476	-13.7429
*	2000	37.544	61.233	285.118	254.502	622.443	551.641	-8.8358
	2500	37.906	80.090	293.532	261.496	641.300	549.300	-5.9600
	3000	38.617	99.197	300.497	267.432	660.407	546.933	-4.0512
	3500	40.095	118.835	306.549	272.596	680.045	544.852	-2.6933
	4000	42.641	139.471	312.056	277.189	700.681	543.552	-1.6782
	4500	46.358	161.672	317.282	281.355	722.882	543.631	-0.8897
	5000	51.123	186.005	322.405	285.204	747.215	545.680	-0.2578
	5500	56.564	212.910	327.530	288.819	774.120	550.163	0.2623
	6000	62.048	242.578	332.689	292.259	803.788	557.290	0.7003
	6500	67.086	274.884	337.858	295.568	836.094		
	7000	71.164	309.499	342.987	298.773	870.709		
	7500	73.898	345.823	347.998	301.888	907.033		
	8000	75.301	383.175	352.819	304.922	944.385		
	8500	75.565	420.934	357.397	307.875	982.144		
	9000	74.936	458.591	361.702	310.747	1019.801		
	9500	73.663	495.763	365.722	313.536	1056.973		
	10000	71.968	532.184	369.458	316.240	1093.394		

*Assigned reference phase change at 1814.00 K,

COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

```
PO2-              TPIS 1989 v1 pt1 p409; pt2 p261.
 3 tpis89 P   1.00O   2.00E   1.00    0.00    0.00 0     62.97311    -597623.751
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 2.702423135D+04 2.939956284D+01 1.162686114D+00 1.599897972D-02-1.979229263D-05
 1.208847527D-08-2.956640480D-12 0.000000000D+00-7.285946270D+04 1.963118182D+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 1.628679152D+06-5.989199980D+03 1.369318836D+01-3.623843790D-03 9.488198340D-07
-1.040308759D-10 4.019033660D-15 0.000000000D+00-3.685959500D+04-5.956796220D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        10613.749
 1.527048695D+08-1.152139645D+05 3.747485230D+01-3.443388910D-03 2.011144470D-07
-5.996871080D-12 7.244612160D-17 0.000000000D+00 8.207935510D+05-2.759665314D+02
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR PO2-

	T deg-K	Cp J/mol-K	H-H298 kJ/mol	S J/mol-K	-(G-H298)/T J/mol-K	H kJ/mol	delta Hf kJ/mol	log K
	0	0.	-10.614	0.	INFINITE	-608.237	-588.000	INFINITE
	298.15	40.517	0.000	249.406	249.406	-597.624	-597.624	103.7681
	300	40.590	0.075	249.657	249.406	-597.549	-597.686	103.1224
*	400	44.365	4.327	261.862	251.045	-593.297	-601.720	77.0173
	500	47.453	8.924	272.108	254.260	-588.699	-604.872	61.2638
	600	49.794	13.792	280.977	257.990	-583.831	-607.854	50.7077
	700	51.528	18.863	288.790	261.843	-578.761	-610.730	43.1311
	800	52.814	24.083	295.759	265.655	-573.541	-613.538	37.4220
	900	53.784	29.415	302.038	269.354	-568.209	-616.303	32.9614
	1000	54.523	34.832	307.745	272.913	-562.791	-619.039	29.3768
	1500	56.477	62.661	330.285	288.511	-534.963	-632.570	18.4965
	2000	57.249	91.114	346.651	301.094	-506.510	-646.158	12.9363
	2500	57.870	119.888	359.490	311.534	-477.735	-660.020	9.5278
	3000	58.720	149.024	370.111	320.437	-448.600	-674.071	7.2065
	3500	59.842	178.654	379.244	328.200	-418.970	-688.120	5.5133
	4000	61.148	208.897	387.319	335.095	-388.727	-701.988	4.2172
	4500	62.502	239.810	394.600	341.308	-357.814	-715.559	3.1892
	5000	63.771	271.384	401.252	346.975	-326.240	-728.790	2.3512
	5500	64.839	303.547	407.382	352.191	-294.077	-741.711	1.6531
	6000	65.624	336.176	413.059	357.030	-261.448	-754.404	1.0612
	6500	66.195	369.142	418.337	361.546	-228.482		
	7000	66.516	402.329	423.255	365.780	-195.295		
	7500	66.635	435.625	427.850	369.766	-161.999		
	8000	66.597	468.938	432.150	373.532	-128.686		
	8500	66.440	502.201	436.183	377.100	-95.422		
	9000	66.199	535.364	439.974	380.489	-62.259		
	9500	65.901	568.391	443.545	383.715	-29.232		
	10000	65.565	601.259	446.917	386.791	3.635		

*Assigned reference phase change at 317.30 K,

Note the following important points:

1. Multiple species are read in sequentially.

2. All species use the same temperature schedule and the same output options.

3. No $\Delta_f H$ or log K values are listed for those temperatures that exceed the range of the reference element coefficients in cap.elms (e.g., S_2F_2 stops at 6000 K in the log K tables because the coefficient data for the reference element sulfur stop at 6000 K, which is also the case for ScO^+ and $PO2^-$).

4. All functions other than $\Delta_f H$ and LOGK are computed and listed to temperatures up to 20 percent beyond the range of the input coefficients (the S_2F_2 MFIG table stops at 7000 K because S_2F_2 coefficient data stops at 6000 K).

Example 4
Ni_3S_2 listing 200 to 10000 K
This example illustrates (1) plot output and (2) gaps in output temperature.

```
'plot' 'joules' 'logk'/
200,100,2000,500,3000/
Ni3S2(a)          Alpha. Bur.Mines Bul.689 1987 p225.JPCRD 1998 Mono.9 p1711.
 1 g12/00 NI  3.00S   2.00    0.00    0.00    0.00 1    240.21220    -217986.400
    200.000    834.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21155.978
-6.710970630D+05 9.870810610D+03-5.338151110D+01 2.311567743D-01-3.933292800D-04
 3.340311640D-07-1.054748249D-10                -7.620212300D+04 2.954015489D+02
Ni3S2(b)          Beta. Bur.Mines Bul.689 1987 p225.
 1 g12/00 NI  3.00S   2.00    0.00    0.00    0.00 2    240.21220    -217986.400
    834.000   1064.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21155.978
-5.072819670D+04 0.000000000D+00 2.665250520D+01-4.426613790D-03 3.885431570D-07
 0.000000000D+00 0.000000000D+00                -3.142142347D+04-1.348956828D+02
Ni3S2(L)          Liquid. Bur.Mines Bul.689 1987 p225.
 1 g12/00 NI  3.00S   2.00    0.00    0.00    0.00 3    240.21220    -217986.400
   1064.000   6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21155.978
 0.000000000D+00 0.000000000D+00 2.274539329D+01 0.000000000D+00 0.000000000D+00
 0.000000000D+00 0.000000000D+00                -2.720113051D+04-1.099086536D+02
```

Example 4 output from CAP

```
 KEYWORDS:  plot   joul   logk
DATA FOR PLOTTING IN FILE plotout

 TEMPERATURE SCHEDULE

    200.000     298.150     300.000     400.000     500.000     600.000
    700.000     800.000     900.000    1000.000    1100.000    1200.000
   1300.000    1400.000    1500.000    1600.000    1700.000    1800.000
   1900.000    2000.000    2500.000    3000.000

                                ***** NOTE *****

  The temperature range of the coefficients read in the standard input (I/O unit 5)
  will be extended by 20 %.  E.g. a range of 300 to 5000 K will be extended to 240
  to 6000 K. The extrapolated data may have large errors. The element data cap.elms
  (I/O unit 13) will NOT be extrapolated when calculating delta H and log K.


                     COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS


     Ni3S2(a)          Alpha. Bur.Mines Bul.689 1987 p225.JPCRD 1998 Mono.9 p1711.
      1 g12/00 NI  3.00S   2.00    0.00    0.00    0.00 1    240.21220    -217986.400
         200.000   834.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21155.978
     -6.710970630D+05 9.870810610D+03-5.338151110D+01 2.311567743D-01-3.933292800D-04
      3.340311640D-07-1.054748249D-10 0.000000000D+00-7.620212300D+04 2.954015489D+02


     Ni3S2(b)          Beta. Bur.Mines Bul.689 1987 p225.
      1 g12/00 NI  3.00S   2.00    0.00    0.00    0.00 2    240.21220    -217986.400
         834.000  1064.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21155.978
     -5.072819670D+04 0.000000000D+00 2.665250520D+01-4.426613790D-03 3.885431570D-07
      0.000000000D+00 0.000000000D+00 0.000000000D+00-3.142142347D+04-1.348956828D+02


     Ni3S2(L)          Liquid. Bur.Mines Bul.689 1987 p225.
      1 g12/00 NI  3.00S   2.00    0.00    0.00    0.00 3    240.21220    -217986.400
        1064.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0        21155.978
      0.000000000D+00 0.000000000D+00 2.274539329D+01 0.000000000D+00 0.000000000D+00
      0.000000000D+00 0.000000000D+00 0.000000000D+00-2.720113051D+04-1.099086536D+02


  THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR Ni3S2(a)    Ni3S2(b)    Ni3S2(L)


       T         Cp        H-H298        S      -(G-H298)/T      H        delta Hf     log K
     deg-K    J/mol-K      kJ/mol     J/mol-K     J/mol-K      kJ/mol      kJ/mol

       0        0.        -21.156       0.        INFINITE   -239.142    -215.960    INFINITE
     200      101.410     -10.855      89.941     144.216    -228.841    -217.518     55.8697
     298.15   117.654       0.000     133.888     133.888    -217.986    -217.986     37.1519
     300      117.870       0.218     134.616     133.890    -217.769    -217.997     36.9164
*    400      127.287      12.509     169.912     138.639    -205.477    -223.097     27.3921
     500      133.726      25.576     199.042     147.891    -192.411    -226.829     21.5233

     600      139.537      39.234     223.928     158.538    -178.753    -230.158     17.5463
*    700      146.973      53.538     245.964     169.480    -164.448    -232.931     14.6631
     800      157.348      68.728     266.231     180.321    -149.258    -233.303     12.4881
     834      161.569      74.149     272.866     183.959    -143.838    -233.224     11.8672
     834      192.548     129.880     339.690     183.959     -88.107    -177.493     11.8672
     900      190.574     142.523     354.280     195.922     -75.464    -175.271     11.0570
    1000      187.606     161.431     374.206     212.774     -56.555    -172.298     10.0484

    1064      185.727     173.378     385.786     222.837     -44.609    -170.681      9.5096
    1064      189.117     193.043     404.268     222.837     -24.944    -151.016      9.5096
    1100      189.117     199.851     410.561     228.878     -18.136    -150.054      9.2677
    1200      189.117     218.762     427.016     244.714       0.776    -147.485      8.6790
    1300      189.117     237.674     442.153     259.327      19.688    -145.164      8.1894
    1400      189.117     256.586     456.169     272.893      38.599    -143.124      7.7757
    1500      189.117     275.498     469.216     285.551      57.511    -141.358      7.4219

    1600      189.117     294.409     481.422     297.416      76.423    -139.870      7.1159
    1700      189.117     313.321     492.887     308.580      95.334    -138.691      6.8485
*   1800      189.117     332.233     503.696     319.123     114.246    -189.274      6.5505
    1900      189.117     351.144     513.921     329.109     133.158    -188.436      6.2621
    2000      189.117     370.056     523.622     338.594     152.070    -187.598      6.0036

    2500      189.117     464.614     565.822     379.976     246.628    -183.406      5.0338

    3000      189.117     559.173     600.302     413.911     341.186    -179.214      4.4020

  *Assigned reference phase change at   631.00 K, 1728.00 K,  388.36 K,
```

Note the following important points:

1. This species experiences two phase transitions below 1100 K. An output line is generated for each phase.
2. Elemental sulfur and elemental nickel are reference elements for this species. Sulfur undergoes two phase transitions in the 300 to 400 K range and melts at 428 K. These phase transitions in this reference element are denoted by the asterisks at 400 and 500 K and a footnote at the end of the log K output table.
3. This run results in an additional file named "plotout" containing T, $C_p^o(T)/R$, [H(T)-H(0)]/RT, $S^o(T)/R$, $-$[G(T)$-$H(0)]/RT, $H^o(T)/RT$ and $-$G(T)/R in columns delineated by spaces. This file (Table ID) facilitates easy plotting by standard plotting programs. Figure 1D shows a plot of C_p^o/R versus T for this species.

TABLE ID.—CONTENTS OF FILE "plotout" FOR EXAMPLE #5

```
4.0000E+02  3.2938E+00  2.1593E+00  4.2120E+00  2.0527E+00  8.0413E-01  3.4079E+00
5.0000E+02  3.5723E+00  2.4136E+00  4.9765E+00  2.5629E+00  1.3295E+00  3.6470E+00
6.0000E+02  3.8543E+00  2.6299E+00  5.6523E+00  3.0224E+00  1.7264E+00  3.9259E+00
7.0000E+02  4.1612E+00  2.8262E+00  6.2689E+00  3.4427E+00  2.0518E+00  4.2171E+00
8.0000E+02  4.5641E+00  3.0167E+00  6.8492E+00  3.8325E+00  2.3391E+00  4.5101E+00
9.0000E+02  5.1809E+00  3.2262E+00  7.4258E+00  4.1996E+00  2.6239E+00  4.8019E+00
1.0000E+03  6.5416E+00  3.4500E+00  8.0005E+00  4.5505E+00  2.9079E+00  5.0925E+00
1.0420E+03  1.0063E+01  3.6353E+00  8.3311E+00  4.6958E+00  3.1151E+00  5.2160E+00
1.0420E+03  1.0064E+01  3.6353E+00  8.3311E+00  4.6957E+00  3.1151E+00  5.2160E+00
1.1000E+03  5.5702E+00  3.8391E+00  8.7384E+00  4.8993E+00  3.3463E+00  5.3921E+00
1.1840E+03  4.9805E+00  3.9043E+00  9.0889E+00  5.1845E+00  3.4465E+00  5.6424E+00
1.1840E+03  4.0751E+00  3.9958E+00  9.1803E+00  5.1845E+00  3.5379E+00  5.6424E+00
1.2000E+03  4.0747E+00  3.9968E+00  9.2350E+00  5.2382E+00  3.5451E+00  5.6899E+00
1.3000E+03  4.1697E+00  4.0059E+00  9.5643E+00  5.5584E+00  3.5889E+00  5.9754E+00
1.4000E+03  4.2832E+00  4.0218E+00  9.8776E+00  5.8558E+00  3.6346E+00  6.2430E+00
1.5000E+03  4.3821E+00  4.0425E+00  1.0176E+01  6.1340E+00  3.6811E+00  6.4954E+00
1.6000E+03  4.4904E+00  4.0670E+00  1.0463E+01  6.3956E+00  3.7282E+00  6.7344E+00
1.6650E+03  4.5583E+00  4.0849E+00  1.0643E+01  6.5579E+00  3.7594E+00  6.8835E+00
1.6650E+03  4.9446E+00  4.1454E+00  1.0703E+01  6.5579E+00  3.8198E+00  6.8835E+00
1.7000E+03  4.9817E+00  4.1623E+00  1.0807E+01  6.6443E+00  3.8434E+00  6.9632E+00
1.8090E+03  5.1234E+00  4.2148E+00  1.1119E+01  6.9046E+00  3.9151E+00  7.2043E+00
1.8090E+03  5.5354E+00  5.1327E+00  1.2037E+01  6.9046E+00  4.8331E+00  7.2043E+00
2.0000E+03  5.5354E+00  5.1712E+00  1.2593E+01  7.4218E+00  4.9001E+00  7.6928E+00
2.5000E+03  5.5354E+00  5.2440E+00  1.3828E+01  8.5841E+00  5.0272E+00  8.8009E+00
3.0000E+03  5.5354E+00  5.2926E+00  1.4837E+01  9.5448E+00  5.1119E+00  9.7255E+00
3.5000E+03  5.5354E+00  5.3273E+00  1.5691E+01  1.0363E+01  5.1724E+00  1.0518E+01
4.0000E+03  5.5354E+00  5.3533E+00  1.6430E+01  1.1076E+01  5.2178E+00  1.1212E+01
4.5000E+03  5.5354E+00  5.3735E+00  1.7082E+01  1.1708E+01  5.2531E+00  1.1829E+01
5.0000E+03  5.5354E+00  5.3897E+00  1.7665E+01  1.2275E+01  5.2813E+00  1.2384E+01
5.5000E+03  5.5354E+00  5.4029E+00  1.8193E+01  1.2790E+01  5.3044E+00  1.2888E+01
6.0000E+03  5.5354E+00  5.4140E+00  1.8674E+01  1.3260E+01  5.3236E+00  1.3351E+01
```

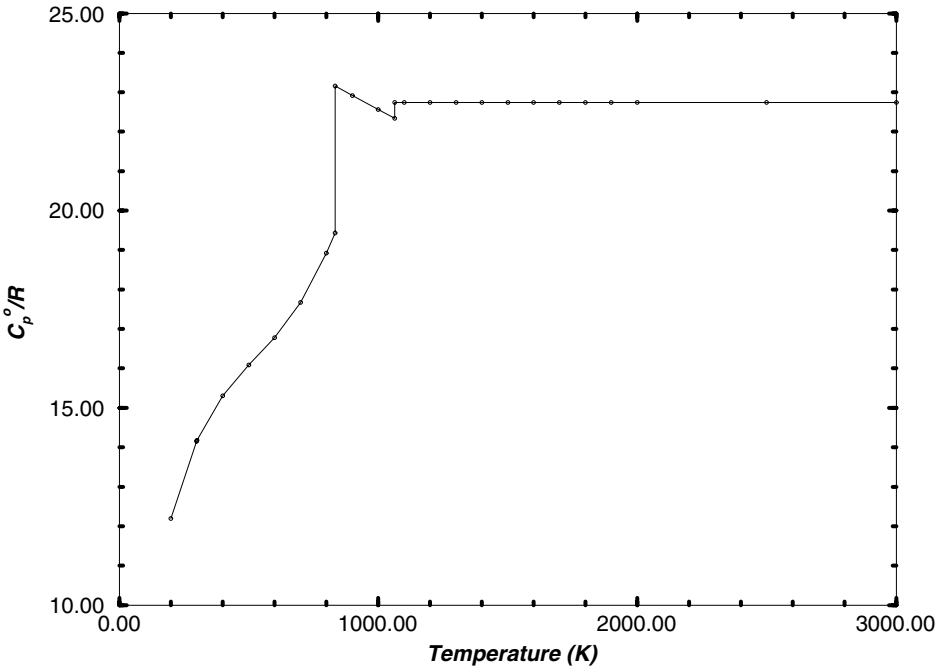

Figure 1D. C_p^o/R for Ni_3S_2(alpha, beta, liquid)

Example 5
Ar, CO, H_2O listing 360R-9000R
This example illustrates the keyword ENGR.

Example 5 input file:

```
'logk' 'mfig','engr' 'nodim' /
360,,900,,1800,,5400,,9000 /
Ar                Ref-Elm. Spec: NSRDS-NBS 35 1971.
 3 g 3/98 AR  1.00    0.00    0.00    0.00    0.00 0     39.94800          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
CO                TPIS 1979 v2 pt1 p25; pt2 p29.
 3 tpis79 C   1.00O   1.00    0.00    0.00    0.00 0   28.0101000    -110535.196
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 1.489045326D+04-2.922285939D+02 5.724527170D+00-8.176235030D-03 1.456903469D-05
-1.087746302D-08 3.027941827D-12 0.000000000D+00-1.303131878D+04-7.859241350D+00
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 4.619197250D+05-1.944704863D+03 5.916714180D+00-5.664282830D-04 1.398814540D-07
-1.787680361D-11 9.620935570D-16 0.000000000D+00-2.466261084D+03-1.387413108D+01
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0         8671.104
 8.868662960D+08-7.500377840D+05 2.495474979D+02-3.956351100D-02 3.297772080D-06
-1.318409933D-10 1.998937948D-15 0.000000000D+00 5.701421130D+06-2.060704786D+03
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
```

Example 5 output file:

```
*******************************************************************************

                 CAP (COEFFICIENTS AND PROPERTIES) PROGRAM
                         NASA GLENN RESEARCH CENTER

   CALCULATES THERMODYNAMIC FUNCTIONS FROM COEFFICIENTS IN THE NASA GLENN FORMAT

*******************************************************************************


 KEYWORDS:  logk   mfig   engr   nodi

 KEYWORD 'ENGR' IMPLIES TEMPERATURES IN SCHEDULE ARE IN DEGREES RANKINE


 TEMPERATURE SCHEDULE

    360.000     536.670     900.000    1800.000    5400.000    9000.000


                                 ***** NOTE *****

  The temperature range of the coefficients read in the standard input (I/O unit 5)
  will be extended by 20 %.  E.g. a range of 300 to 5000 K will be extended to 240
  to 6000 K. The extrapolated data may have large errors. The element data cap.elms
  (I/O unit 13) will NOT be extrapolated when calculating delta H and log K.


                  COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS


    Ar                Ref-Elm. Spec: NSRDS-NBS 35 1971.
     3 g 3/98 AR  1.00    0.00    0.00    0.00    0.00 0     39.94800          0.000
        200.000  1000.000 7 -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 0.000000000D+00-7.453750000D+02 4.379674910D+00
       1000.000  6000.000 7 -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 0.000000000D+00-7.449939610D+02 4.379180110D+00
       6000.000 20000.000 7 -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 0.000000000D+00-5.078300340D+06 1.465298484D+03


 THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR Ar

      Assigned H(T)/R at   0.00 Rankine =   -1341.675 Rankine

    T         Cp/R      (H-H0)/RT       S/R      -(G-H0)/RT       H/RT         -G/RT

  360.00     2.50000    2.5000001   17.6254683   15.1254683    -1.2268750    18.8523433
  536.67     2.50000    2.5000000   18.6236667   16.1236667     0.0000000    18.6236667
  900.00     2.50000    2.5000000   19.9161952   17.4161951     1.0092500    18.9069452
 1800.00     2.50000    2.5000000   21.6490631   19.1490631     1.7546250    19.8944381
 5400.00     2.50000    2.5000000   24.3955938   21.8955938     2.2515417    22.1440522
 9000.00     2.50000    2.5000000   25.6726579   23.1726579     2.3509250    23.3217329


 THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR Ar

    Assigned H(T) at    0.00 Rankine =     -66.697 BTU/lb

     T           Cp          H-H0         S          -(G-H0)         H           -G
  Rankine    BTU/lb-deg      BTU/lb    BTU/lb-deg     BTU/lb        BTU/lb       BTU/lb

  360.00      0.12428      44.7406     0.876193     270.6890      -21.9565      337.3861
  536.67      0.12428      66.6971     0.925816     430.1604        0.0000      496.8575
  900.00      0.12428     111.8515     0.990070     779.2111       45.1545      845.9082
 1800.00      0.12428     223.7030     1.076214    1713.4813      157.0060     1780.1784
 5400.00      0.12428     671.1091     1.212748    5877.7327      604.4120     5944.4297
 9000.00      0.12428    1118.5151     1.276234   10367.5873     1051.8181    10434.2844
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR Ar

T Rankine	Cp BTU/lb-deg	H-H537 BTU/lb	S BTU/lb-deg	-(G-H537)/T BTU/lb-deg	H BTU/lb	delta Hf BTU/lb	log K
0	0.	-66.697	0.	INFINITE	-66.697	0	INFINITE
360	0.1243	-21.956	0.876	0.937	-21.956	0	0
536.67	0.1243	0.000	0.926	0.926	0.000	0	0
900	0.1243	45.154	0.990	0.940	45.154	0	0
1800	0.1243	157.006	1.076	0.989	157.006	0	0
5400	0.1243	604.412	1.213	1.101	604.412	0	0
9000	0.1243	1051.818	1.276	1.159	1051.818	0	0

COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

```
  CO                TPIS 1979 v2 pt1 p25; pt2 p29.
   3 tpis79 C   1.00O   1.00    0.00    0.00    0.00 0     28.01010    -110535.196
      200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8671.104
    1.489045326D+04-2.922285939D+02 5.724527170D+00-8.176235030D-03 1.456903469D-05
   -1.087746302D-08 3.027941827D-12 0.000000000D+00-1.303131878D+04-7.859241350D+00
     1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8671.104
    4.619197250D+05-1.944704863D+03 5.916714180D+00-5.664282830D-04 1.398814540D-07
   -1.787680361D-11 9.620935570D-16 0.000000000D+00-2.466261084D+03-1.387413108D+01
     6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8671.104
    8.868662960D+08-7.500377840D+05 2.495474979D+02-3.956351100D-02 3.297772080D-06
   -1.318409933D-10 1.998937948D-15 0.000000000D+00 5.701421130D+06-2.060704786D+03
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CO

Assigned H(T)/R at 0.00 Rankine = -25806.853 Rankine

T	Cp/R	(H-H0)/RT	S/R	-(G-H0)/RT	H/RT	-G/RT
360.00	3.50098	3.4956207	22.3744710	18.8788502	-68.1900829	90.5645539
536.67	3.50488	3.4978641	23.7728765	20.2750124	-44.5891415	68.3620181
900.00	3.58334	3.5123929	25.5982236	22.0858307	-25.1618886	50.7601122
1800.00	3.99047	3.6512651	28.2086216	24.5573565	-10.6858757	38.8944972
5400.00	4.47471	4.0972618	32.9086030	28.8113413	-0.6817851	33.5903882
9000.00	4.57785	4.2709476	35.2212063	30.9502587	1.4035194	33.8176869

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CO

Assigned H(T) at 0.00 Rankine = -1829.678 BTU/lb

T Rankine	Cp BTU/lb-deg	H-H0 BTU/lb	S BTU/lb-deg	-(G-H0) BTU/lb	H BTU/lb	-G BTU/lb
360.00	0.24822	89.2209	1.586326	481.8565	-1740.4576	2311.5350
536.67	0.24849	133.0914	1.685472	771.4507	-1696.5871	2601.1292
900.00	0.25405	224.1224	1.814887	1409.2757	-1605.5560	3238.9542
1800.00	0.28292	465.9675	1.999961	3133.9629	-1363.7110	4963.6413
5400.00	0.31725	1568.6541	2.333185	11030.5448	-261.0243	12860.2232
9000.00	0.32456	2725.2508	2.497146	19749.0640	895.5723	21578.7425

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR CO

T Rankine	Cp BTU/lb-deg	H-H537 BTU/lb	S BTU/lb-deg	-(G-H537)/T BTU/lb-deg	H BTU/lb	delta Hf BTU/lb	log K
0	0.	-133.091	0.	INFINITE	-1829.678	-1746.894	INFINITE
360	0.2482	-43.871	1.586	1.708	-1740.458	-1708.234	33.5696
536.67	0.2485	0.000	1.685	1.685	-1696.587	-1696.587	24.0319
900	0.2541	91.031	1.815	1.714	-1605.556	-1688.578	16.2370
1800	0.2829	332.876	2.000	1.815	-1363.711	-1719.017	10.4619
5400	0.3173	1435.563	2.333	2.067	-261.024	-1956.758	6.4043
9000	0.3246	2592.159	2.497	2.209	895.572	-2291.968	5.4566

COEFFICIENTS FOR FITTED THERMODYNAMIC FUNCTIONS

```
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     18.01528    -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
```

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR H2O

Assigned H(T)/R at 0.00 Rankine = -54496.797 Rankine

T	Cp/R	(H-H0)/RT	S/R	-(G-H0)/RT	H/RT	-G/RT
360.00	4.01100	3.9817473	21.1049377	17.1231904	-147.3982450	168.5031827
536.67	4.03965	3.9952428	22.7107930	18.7155502	-97.5509536	120.2617466
900.00	4.23655	4.0480662	24.8396421	20.7915759	-56.5039307	81.3435728
1800.00	4.96614	4.3186473	27.9916330	23.6729857	-25.9573512	53.9489842
5400.00	6.83426	5.5149536	34.5172068	29.0022532	-4.5770459	39.0942527
9000.00	7.34198	6.1570656	38.1436667	31.9866011	0.1018659	38.0418008

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR H2O

Assigned H(T) at 0.00 Rankine = -6007.370 BTU/lb

T Rankine	Cp BTU/lb-deg	H-H0 BTU/lb	S BTU/lb-deg	-(G-H0) BTU/lb	H BTU/lb	-G BTU/lb
360.00	0.44215	158.0118	2.326470	679.5174	-5849.3577	6686.8869
536.67	0.44530	236.3545	2.503489	1107.1929	-5771.0150	7114.5624
900.00	0.46701	401.6090	2.738159	2062.7343	-5605.7605	8070.1038
1800.00	0.54743	856.9068	3.085614	4697.1984	-5150.4627	10704.5680
5400.00	0.75336	3282.8345	3.804951	17263.8982	-2724.5350	23271.2677
9000.00	0.80933	6108.4308	4.204708	31733.9382	101.0613	37741.3077

THERMODYNAMIC FUNCTIONS CALCULATED FROM COEFFICIENTS FOR H2O

T Rankine	Cp BTU/lb-deg	H-H537 BTU/lb	S BTU/lb-deg	-(G-H537)/T BTU/lb-deg	H BTU/lb	delta Hf BTU/lb	log K
0	0.	-236.355	0.	INFINITE	-6007.370	-5701.712	INFINITE
360	0.4421	-78.343	2.326	2.544	-5849.358	-5748.903	60.7903
536.67	0.4453	0.000	2.503	2.503	-5771.015	-5771.015	40.0453
900	0.4670	165.255	2.738	2.555	-5605.760	-5818.757	22.8831
1800	0.5474	620.552	3.086	2.741	-5150.463	-5914.900	10.0592
5400	0.7534	3046.480	3.805	3.241	-2724.535	-6012.787	1.3492
9000	0.8093	5872.076	4.205	3.552	101.061	-6044.104	-0.4080

Note the following important points:

1. The keyword ENGR requires that the temperature schedule (supplied by the user) must be in degrees Rankine.

2. Output tables are listed in British thermal units per pound (BTU/lb) and British thermal units per pound-degree (BTU/lb-°) Rankine with temperatures in Rankine.

3. The NASA Glenn coefficients are for temperatures in degrees K. These coefficients are not changed for Rankine runs.

4. The keywords JOULES and CAL are ignored when ENGR has been specified.

References

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13. ABSTRACT ***(Maximum 200 words)***

For several decades the NASA Glenn Research Center has been providing a file of thermodynamic data for use in several computer programs (Gordon and McBride, 1994; McBride and Gordon, 1996; and Radhakrishnan and Bittker, 1994). These data are in the form of least-squares coefficients that have been calculated from tabular thermodynamic data by means of the NASA Properties and Coefficients (PAC) program (McBride and Gordon, 1992). The source thermodynamic data are obtained from the literature or from standard compilations (e.g., Chase, 1998; Gurvich et al., 1989, 1991, 1996; Barin, 1989; and TRC Thermodynamic Tables). Most gas-phase thermodynamic functions are calculated by the authors from molecular constant data using ideal gas partition functions. The Coefficients and Properties (CAP) program described in this report permits the generation of tabulated thermodynamic functions from the NASA least-squares coefficients. CAP provides considerable flexibility in the output format, the number of temperatures to be tabulated, and the energy units of the calculated properties. This report provides a detailed description of input preparation, examples of input and output for several species, and a listing of all species in the current NASA Glenn thermodynamic data file.

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Heats of formation; CEA; McBride; Gordon; Thermodynamics; Thermodynamic properties; NASA; NASA Lewis; Specific heat; NASA Glenn; Enthalpy; Entropy; Heat capacity

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