



# NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species

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Space Administration

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The Aerospace Propulsion and Power Program at  
NASA Glenn Research Center sponsored this work.

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## **In Memoriam**



### **Sanford Gordon**

1920 to 2001

This report is dedicated to the memory of Sanford Gordon, who pioneered the application of computers for calculating thermodynamic properties and for using these properties to model the behavior of reacting systems.



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## Summary

This report documents the library of thermodynamic data used with the NASA Glenn computer program CEA (Chemical Equilibrium with Applications). This library, containing data for over 2000 solid, liquid, and gaseous chemical species for temperatures ranging from 200 to 20 000 K, is available for use with other computer codes as well. The data are expressed as least-squares coefficients to a seven-term functional form for  $C_p^o(T)/R$  with integration constants for  $H^o(T)/RT$  and  $S^o(T)/R$ . The NASA Glenn computer program PAC (Properties and Coefficients) was used to calculate thermodynamic functions and to generate the least-squares coefficients. PAC input was taken from a variety of sources. A complete listing of the database is given along with a summary of thermodynamic properties at 0 and 298.15 K.

## Introduction

Thermodynamic data for individual species are required in many applications involving chemical reactions. For over 50 years the NASA Lewis (now Glenn) Research Center has been compiling and disseminating thermodynamic data for use in its chemical equilibrium programs. These data, widely used by the thermodynamic community, have grown from 42 species to the current 2000.

For calculation purposes, the use of thermodynamic data in the form of simple empirical equations has some obvious advantages. First, it makes tabular interpolations unnecessary; second, it permits analytical integrations; and, third, it condenses all the tabulated information into a few constants that accurately reproduce the many thermodynamic data points.

Earlier versions of the NASA Lewis chemical equilibrium computer programs (Gordon et al., 1971, Svehla et al., 1973, Gordon et al., 1976, Gordon et al., 1984,

Gordon et al., 1988, and McBride et al., 1994) used a fourth-order polynomial as an empirical representation of  $C_p^o(T)/R$  over a temperature range of 300 to 5000 K. The final library of data using this form contained 1130 species documented in NASA TM-4513 (McBride et al., 1993b). For the data in the current report, two terms involving  $T^{-1}$  and  $T^{-2}$  were added for more accuracy over wider temperature ranges.

A new format was selected that would not only accommodate these two new constants but also allow for revisions and expansions in the future. Features of the new format and how they were used in this report are as follows:

(1) Up to eight constants can be used in the empirical equation for  $C_p^o(T)/R$ . Only seven were used for the data reported here.

(2) Variable temperature intervals can be used. This new feature was helpful in obtaining good fits for condensed species, which often have irregularly shaped curves and variable transition points. However, standard temperature intervals were used for gases. With a few exceptions, fixed intervals fit the thermodynamic functions for gases accurately.

(3) There is space for comments and references.

(4) The chemical formula may now contain up to five unique atoms. The previous format allowed for only four atoms.

(5) Variable and noninteger temperature exponents are now permitted in the empirical equation for  $C_p^o(T)/R$ . We used the exponents  $-2$ ,  $-1$ ,  $0$ ,  $1$ ,  $2$ ,  $3$ , and  $4$ .

(6) The new format is easier to read. For convenience, values are also given for the molecular weight, heat of formation, and  $H^o(298.15) - H^o(0)$ .

All symbols used in this report are listed and defined in appendix A. Appendix B contains tables summarizing the thermodynamic data at 0 and 298.15 K. Appendix C gives a description of the particular format used for the database, and appendix D is a complete listing of the NASA Glenn coefficient data as of the date of this report.

The data for individual species are updated as new measurements and estimates appear in the literature. The database is distributed freely via a request form on the internet at <http://www.grc.nasa.gov/WWW/CEAWeb/>.

## Standard States, Reference States, and Fundamental Constants

The symbols and definitions follow the recommendations of Cox (1982). All data in this report are for species in their standard state at the specified temperature. For gases, this is the ideal gas at the standard pressure, 1 bar. For condensed species, the standard state is the pure crystalline or liquid substance at the standard pressure, 1 atm. All thermodynamic properties are molar quantities.

In order for heats of formation to be unambiguously related to specific reactions, a set of reference states must be specified for the chemical elements. The reference state of the elements is generally taken to be the thermodynamically stable state at 298.15 K. For those elements which are gases at 298.15 K and 1 bar, the reference state is taken as gaseous over the entire temperature range. For species that are condensed at 298.15 K, the entire range is taken to be condensed with transitions between various phases. In appendix D, these reference species have either 'Ref-elm' or 'Ref-species' following their name.

Fundamental constants were taken from Cohen et al. (1987). The values used for the molar gas constant  $R$ , the Sackur-Tetrode constant  $S_o/R$ , the second radiation constant  $c_2$ , and the electron mass  $m_e$  are given in the symbol list in appendix A. Some thermodynamic functions taken from the literature were calculated using values of  $R$  and Sackur-Tetrode constants different from those selected for this report. In these cases, corrections were made to the thermodynamic functions to adjust for the differences. Corrections were made to entropy and Gibbs energy values that had been previously calculated using 1 atm for the standard state pressure rather than 1 bar.

The atomic weights were taken from Coplen (1996). These weights are given in atomic mass units, u, based on  $^{12}\text{C} = 12 \text{ u}$ .

## Empirical Equations for Fitting Thermodynamic Functions

Thermodynamic data for many individual species can be conveniently stored for use with computer programs

in the form of coefficients associated with equations that reproduce the data. The following dimensionless form was chosen for this report:

$$C_p^o(T)/R = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (1)$$

Enthalpy and entropy are obtained by integrating  $C_p^o(T)$  and  $C_p^o(T)/T$ , respectively, with respect to  $T$ :

$$H^o(T)/RT = -a_1 T^{-2} + a_2 \ln T/T + a_3 + a_4 T/2 + a_5 T^2/3 + a_6 T^3/4 + a_7 T^4/5 + b_1/T \quad (2)$$

$$S^o(T)/R = -a_1 T^{-2}/2 - a_2 T^{-1} + a_3 \ln T + a_4 T + a_5 T^2/2 + a_6 T^3/3 + a_7 T^4/4 + b_2 \quad (3)$$

where  $b_1$  and  $b_2$  are integration constants. These equations have been found to accurately reproduce the thermodynamic quantities over a wide temperature range.

## Assigned Enthalpy Values

For each species, heats of formation (and, when applicable, heats of transition) were combined with sensible heats,  $H^o(T) - H^o(298.15)$ , to give the assigned enthalpies,  $H^o(T)$ . By definition

$$H^o(T) \equiv H^o(298.15) + [H^o(T) - H^o(298.15)] \quad (4)$$

We arbitrarily assign  $H^o(298.15) = \Delta_f H^o(298.15)$ . The above equation then becomes

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

In general,  $H^o(T)$  will not equal  $\Delta_f H^o(T)$  except at 298.15 K. Similarly, for the  $H^o(0)$  values listed in tables B1 and B2 in appendix B,

$$H^o(0) = \Delta_f H^o(298.15) - [H^o(298.15) - H^o(0)] \quad (6)$$

All reference elements and the reference species electron gas have assigned enthalpy values,  $H^o(298.15)$ , equal to zero.

Assigned enthalpies for reactants are listed in table B3 in appendix B. For noncryogenic reactants, assigned enthalpies are given at 298.15 K. For cryogenic liquids, assigned enthalpies are given at their boiling points

instead of 298.15 K. These are obtained by subtracting the following values from the heat of formation of the gas at 298.15 K: (1) the sensible heat of the ideal gas at 298.15 K relative to the boiling point, (2) the relative enthalpy of the ideal gas to the real gas at the boiling point, and (3) the heat of vaporization at the boiling point.

## Heats of Formation and Equilibrium Constants

At any temperature, values of  $\Delta_f H^\circ$  and  $\log_{10} K$  may be calculated for the formation of a species from its constituent elements in their assigned reference states. The following is an example of how these properties can be calculated for CO(g) at 1000 K:

$$\Delta_f H^\circ(1000) = H^\circ(1000) \text{ CO(g)} - H^\circ(1000) \text{ C(graphite)} - \frac{1}{2} H^\circ(1000) \text{ O}_2(\text{g}) \quad (7)$$

$$\Delta_f G^\circ(1000) = G^\circ(1000) \text{ CO(g)} - G^\circ(1000) \text{ C(graphite)} - \frac{1}{2} G^\circ(1000) \text{ O}_2(\text{g}) \quad (8)$$

By definition,

$$\log_{10} K \equiv -\Delta_f G^\circ(T)/(2.3025851 RT) \quad (9)$$

## Properties and Coefficients (PAC) Programs

The NASA Glenn computer program PAC99 was used to convert molecular constants and thermodynamic data into the coefficient form described in appendix C. PAC99 is the latest in a series of FORTRAN programs that generate data in the format required by CEA. It is an expanded version of PAC91 (McBride et al., 1992). The expansion includes new techniques for calculating properties for atomic species (Gordon et al., 1999), increased dimensions for larger molecules, and the capacity to use more parameters in internal rotor calculations. The following sections discuss the tasks performed by this program.

### Thermodynamic Properties

Thermodynamic properties may be read in either as thermodynamic functions or as coefficients. A method

for extrapolating these data to higher temperatures is provided. For gases, PAC99 provides several methods for calculating thermodynamic functions from molecular data.

The calculation methods used for monatomic gases are outlined in Gordon et al. (1999). For polyatomic species, six closed-form calculation methods are available (McBride et al., 1992). All were used in this report. All use a rigid-rotor harmonic-oscillator base with corrections for anharmonicities, vibration-rotation interactions, rotational stretching, low-temperature quantum rotation, Fermi and Darling-Dennison resonance, and internal rotation. The Darling-Dennison resonance and some low-temperature quantum corrections (Gurvich et al., 1989) have been added since PAC91. The internal rotor calculations were also expanded to use more potential and rotational constants (Lewis et al., 1972, and Zeleznik, 2002). Equilibrium mixtures of isomers were calculated by summing the partition functions for each conformer. PAC99 calculates tables of thermodynamic functions including  $\Delta_f H^\circ$  and  $\log_{10} K$  with an option to do a least-squares fit of the data.

### Least-Squares Fit

Most coefficients in equations (1) to (3) were obtained using the least-squares fit feature in PAC99. For gases, the temperature ranges for these fits are split into three fixed intervals: 200 to 1000 K (298.15 to 1000 K for ions), 1000 to 6000 K, and for some simple molecules, 6000 to 20 000 K. For condensed species, the temperature ranges are variable, with each phase having its own set of coefficients. The fits were subject to the following constraints:

- (1) An exact fit at 298.15 K.
- (2) Coefficients for two contiguous intervals yield the same functional values at the common point.
- (3) The difference in Gibbs energy is zero between condensed phases.
- (4) Generally  $C_p^\circ(T)/R$ ,  $[H^\circ(T) - H^\circ(0)]/RT$ , and  $S^\circ(T)$  were fit simultaneously as suggested by Zeleznik et al. (1961). However, this method was not used for monatomic species, where electronic levels were truncated with a temperature-dependent cutoff technique (Gordon et al., 1999). For these cases, the least-squares fit was on  $C_p^\circ(T)/R$  only.

Generally for intervals where  $C_p^\circ(T)/R$  is constant, a least-squares fit was not done.

## Data Sources

Each species within the coefficient data file (app. D) contains abbreviated references to the data used to generate those coefficients. Complete reference citations, ordered by first author's last name and year, are listed at the end of this report.

Heats of formation were often obtained indirectly from other values (e.g., dissociation energies). This required the use of additional thermodynamic data. Generally, the supporting data were taken from the NASA database, otherwise the references are indicated.

For condensed species, either thermodynamic functions or fitted coefficients were taken directly from the references listed. For most gases the functions were calculated with the PAC99 program using molecular data from the cited references and any of several calculation techniques. However, for diatomic gases most of the functions were taken directly from the Gurvich references because they used a direct summation method not currently part of PAC99. If molecular constants for excited electronic states of diatomic and polyatomic gases were not available in the source reference, they were taken from another electronic state, usually the ground state.

Calculation techniques for monatomic species are described in Gordon et al. (1999). When thermodynamic functions for a gas were taken directly from the literature and were not given to high enough temperatures (e.g., 6000 or 20 000 K), they were extrapolated by the method described in Wilhoit (1975). Extrapolations were done in order to provide reasonable values outside the temperature range of the original data, which is important when CEA iterates on  $T$ . During the iteration,  $T$  may be temporarily out of range of the original data, resulting in thermodynamic properties so inaccurate that convergence is impossible.

## Thermodynamic Properties at 0 and 298.15 K

A summary of the thermodynamic properties at 0 and 298.15 K is given in appendix B. There are three tables:

Table B1.—Thermodynamic Properties for Gases at 0 and 298.15 K

Table B2.—Thermodynamic Properties for Condensed Species at 0 and 298.15 K

Table B3.—Assigned Enthalpies for Species That Are Used in CEA as Reactants Only

Note that reactants-only species with coefficients appear not only in table B3 but also in table B1 or B2. The thermodynamic quantities at 298.15 K were calculated from the coefficients. Since the least-squares fits are constrained to fit these values, the listed quantities match the source values. The third table lists assigned enthalpies and associated temperatures, molecular weights, and stoichiometric coefficients for species in the reactant-only class. No other thermodynamic quantities are listed in this table because coefficients are not available for most of the species.

## Thermodynamic Coefficients Data

Appendix D lists the thermodynamic data as distributed in a file called thermo.inp. Appendix C discusses the format of this file. It shows the exact placement of names, references and comments, reference-date codes, chemical formula, molecular weights, heats of formation,  $H^o(T) - H^o(0)$  values, temperature ranges, number of temperature intervals, phase code, and coefficients.

The following sections contain general comments on species names, data order, and miscellaneous information useful in interpreting the database. Each line of data is referred to as a record.

## Species Names

The first 15 characters in the first record are reserved for the species name, usually the chemical formula. Longer names are often truncated. The letter "l," which is normally lowercase, has been replaced with uppercase "L" to avoid confusion with the number "1." Condensed phases designated as  $\alpha$ ,  $\beta$ ,  $\gamma$ , or  $\delta$  are called  $a$ ,  $b$ ,  $c$ , or  $d$  because FORTRAN does not allow Greek letters. Similarly, numbers normally shown as subscripts are printed on the main line for the same reason.

## References

References and comments follow the species name in record 1. References are usually depicted by the first author's last name and the year of publication. An exception is for the TRC (Thermodynamic Research Center) looseleaf tables, where page and table date are used. Comments are abbreviated to fit the space available. When the heat of formation is taken from a separate reference, it is indicated as "Hf:". Reference elements

or reference species used for heats of formation are indicated by “Ref-Elm.” or “Ref-Species.”

## Species Order

The data are divided into three categories and are listed in the following order:

- (1) Gases used in CEA as possible products and reactants (pp. 45–210)
- (2) Condensed species used in CEA as possible products and reactants (pp. 210–276)
- (3) Species that may be used only as reactants in CEA (e.g., air or Jet-A) (pp. 276–280)

Within the first two categories, the species are listed alphabetically according to the chemical formula given on the second record. The reactants-only set is listed alphabetically by name. This set is separated from the first two by a single record “END PRODUCTS” (see p. 276).

For condensed species with multiple phases, individual phases are listed in increasing order according to their temperature ranges. Consecutive phases are numbered consecutively starting with “1” in column 52 in record 2. See appendix C.

## Reference-Date Codes

Record 2 contains a six-character code designating a reference and date as defined at the beginning of appendix D. The alphabetic part of the code represents a large compilation of data (e.g., “j” for JANAF or “g” for Glenn Research Center). The “g” was used if the PAC99 input data either (1) came from mixed sources, (2) came from a source not coded, (3) were molecular constants where no thermodynamic functions were given in the source, or (4) were molecular constants with a calculation method differing from the method used by the source.

## Temperature Ranges

For nonionic gases, the temperature range of the fitted data is either 200 to 6000 K, or 200 to 20 000 K. For ionic gases, the starting temperature is 298.15 K. Only the electron gas, monatomic species, and simple molecules (e.g., CO, CO<sub>2</sub>, N<sub>2</sub>, NO, and O<sup>+</sup>) have been fitted to 20 000 K. For gases, there is a breakpoint in the fit at

1000 K. For gases fitted to 20 000 K, there is an additional breakpoint at 6000 K. Each temperature range is listed in the record preceding the corresponding coefficients. For condensed species, the temperature ranges and breakpoints are set according to the data and accuracy of the fits.

## Using the Coefficients to Obtain Thermodynamic Functions

The NASA Glenn database can be used to obtain listings of thermodynamic functions, either interactively online with the Properties From Coefficients (PFC) computer program or by use of the Coefficients and Properties (CAP) computer program (Zehe et al., 2001).

The PFC interactive program provides a Periodic Table of the Elements from which the user selects constituent atoms for the species to be tabulated. PFC presents a list of all species in the database containing those elements. The user selects the species of interest and the temperature schedule to be used. PFC lists the current NASA coefficients for those species and uses them to create a table of  $C_p^o(T)$ ,  $H^o(T) - H^o(298.15)$ ,  $S^o(T)$ ,  $-[G^o(T) - H^o(T)]/T$ ,  $H^o(T)$ ,  $\Delta H_f^o(T)$ , and  $\log K(T)$  at each temperature in the schedule. Data are also listed for 0 K, 298.15 K, and for all phase changes within the temperature schedule. PFC can be accessed directly at <http://cea.grc.nasa.gov> or from the CEA Web site <http://www.grc.nasa.gov/WWW/CEAWeb/> with the selection “Get Properties from NASA Coefficients (PFC).”

The CAP program allows users to tabulate thermodynamic functions from the NASA Glenn coefficients without being connected to the Internet. Thermodynamic functions may be tabulated in SI units, in chemical units (calories and kelvin), or in “engineering” units (Btu/lb-mol and Btu/lb-mol-°R). An option allows the user to generate a file listing temperatures and thermodynamic functions in column format for easy plotting. The program is described in NASA/TP—2001-210959 (Zehe et al., 2001). CAP and the NASA Glenn database are available via a request form at the CEA Web site <http://www.grc.nasa.gov/WWW/CEAWeb/>.

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## Appendix A Symbols

$a_i$ ( $i = 1, 7$ )	temperature coefficients in eqs. (1), (2), and (3)	$H^o(0)$	chemical energy (molar enthalpy) at 0 K for standard state
$b_1, b_2$	integration constants defined by eqs. (2) and (3)	$H^o(298.15)$	assigned molar enthalpy at 298.15 K for standard state (equals $\Delta_f H^o(298.15)$ )
$C_p^o(T)$	molar heat capacity at constant pressure at temperature $T$ for standard state, eq. (1)	$K$	equilibrium constant
$c_2$	second radiation constant, 1.438769 cm-K	$m_e$	electron mass, 0.000548579903 u
$G^o(T)$	either $[G^o(T) - H^o(0)] + H^o(0)$ or $[G^o(T) - H^o(298.15)] + H^o(298.15)$	$R$	universal gas constant, 8.314510 J/(mol-K)
$G^o(T) - H^o(0)$	molar Gibbs energy at temperature $T$ relative to enthalpy at 0 K for standard state	$S^o(T)$	entropy at temperature $T$ 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	$S_o/R$	Sackur-Tetrode constant for $p_o = 1$ bar, -1.151693
$H^o(T)$	either $[H^o(T) - H^o(0)] + H^o(0)$ or $[H^o(T) - H^o(298.15)] + H^o(298.15)$	$T$	temperature, K
$H^o(T) - H^o(0)$	molar enthalpy at temperature $T$ relative to molar enthalpy at 0 K for standard state	$\Delta_f G^o(T)$	molar Gibbs energy of formation of a substance at temperature $T$ from its reference species in their 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 species in their standard state





## Appendix B

### Thermodynamic Properties at 0 and 298.15 K

This appendix contains three tables summarizing the properties of the species in thermo.inp (app. D) at 0 and 298.15 K. Table B1 is for all gaseous species that have coefficients including those used in the NASA program CEA (Chemical Equilibrium with Applications) for reactants-only species. Table B2 lists data for all condensed species. Table B3 summarizes information for all the reactants-only species whether or not they have coefficients.

For cryogenic liquids in this last table, assigned enthalpies  $H^o(T)$  are given at their boiling points rather than 298.15 K. For more details on assigned enthalpies see the section “Assigned Enthalpy Values.”

**TABLE B1.—THERMODYNAMIC PROPERTIES FOR GASES AT 0 AND 298.15 K**

Species name	Molecular weight	$H^o(0)$ kJ/mol	$\Delta_f H^o(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^o(T)$ kJ/mol	$C_p^o(T)$ J/K-mol	$H^o(T) - H^o(0)$ kJ/mol	$S^o(T)$ J/K-mol
e-	5.4858-04	-6.197	-6.197	0.000	20.786	6.197	20.979
Ag	107.86820	278.703	284.448	284.900	20.786	6.197	172.998
Ag+	107.86765	1015.896	1015.444	1022.094	20.792	6.198	167.236
Ag-	107.86875	146.881	158.824	153.079	20.786	6.197	167.235
AL	26.98154	323.081	327.621	330.000	21.391	6.919	164.555
AL+	26.98099	906.818	905.160	913.015	20.786	6.197	149.952
AL-	26.98209	274.334	285.071	281.090	20.960	6.756	168.137
ALBr	106.88554	4.754	21.554	14.325	35.618	9.571	239.635
ALBr2	186.78954	-154.060	-125.000	-140.662	53.256	13.398	312.236
ALBr3	266.69354	-428.420	-387.100	-410.477	75.372	17.943	348.026
ALC	38.99224	673.225	678.819	682.284	33.218	9.058	225.918
ALC2	51.00294	663.353	670.000	675.616	47.818	12.263	252.941
ALCL	62.43424	-60.331	-51.200	-51.007	34.661	9.323	227.961
ALCL+	62.43369	852.695	855.628	861.849	33.794	9.154	232.190
ALCL2	97.88694	-253.721	-240.000	-240.874	51.566	12.847	290.374
ALCL3	133.33964	-601.080	-582.768	-584.679	71.537	16.401	313.089
ALF	45.97994	-272.953	-264.000	-264.060	31.937	8.892	215.162
ALF+	45.97939	683.421	686.176	692.234	31.155	8.813	220.068
ALFCL	81.43264	-448.543	-435.000	-436.410	48.267	12.133	282.721
ALFCL2	116.88534	-807.134	-789.000	-791.395	68.808	15.738	311.383
ALF2	64.97834	-643.365	-630.000	-631.764	45.418	11.601	264.924
ALF2-	64.97889	-864.563	-845.000	-853.231	44.746	11.332	257.271
ALF2CL	100.43104	-1013.956	-996.000	-999.128	65.546	14.828	298.135
ALF3	83.97675	-1223.321	-1205.543	-1209.277	62.199	14.044	276.674
ALF4-	102.97570	-1968.388	-1940.000	-1951.601	80.986	16.787	293.563
ALH	27.98948	240.583	249.357	249.251	29.371	8.668	187.863
ALHCL	63.44218	-0.365	13.000	10.522	42.023	10.887	257.237
ALHCL2	98.89488	-364.955	-347.000	-351.279	60.517	13.676	288.762
ALHF	46.98788	-193.187	-180.000	-182.614	39.732	10.572	245.469
ALHFCL	82.44058	-567.777	-550.000	-555.245	56.969	12.533	278.249
ALHF2	65.98628	-777.599	-760.000	-765.299	53.676	12.300	263.716
ALH2	28.99742	266.684	279.692	276.775	35.773	10.091	213.316
ALH2CL	64.45012	-117.599	-100.000	-106.345	47.528	11.253	251.100
ALH2F	47.99582	-327.421	-310.000	-316.656	44.221	10.765	238.744
ALH3	30.00536	118.486	135.728	128.896	40.057	10.411	206.579

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
ALI	153.88601	57.644	68.782	67.395	36.135	9.751	247.840
ALI2	280.79048	-47.736	-30.000	-33.813	54.635	13.923	328.828
ALI3	407.69495	-210.334	-186.000	-191.330	77.474	19.004	373.832
ALN	40.98828	429.564	438.439	438.829	32.417	9.265	228.437
ALO	42.98094	58.531	67.411	67.319	30.884	8.788	218.389
ALO+	42.98039	983.903	986.586	992.993	33.135	9.090	230.978
ALO-	42.98149	-281.666	-266.589	-272.922	30.335	8.745	211.945
ALOCL	78.43364	-313.471	-300.000	-301.565	50.368	11.906	252.377
ALOCL2	113.88634	-418.061	-400.000	-402.309	68.896	15.752	316.893
ALOF	61.97934	-583.293	-570.000	-572.290	46.787	11.003	238.965
ALOF2	80.97774	-787.705	-770.000	-773.650	62.253	14.055	291.335
ALOF2-	80.97829	-986.367	-962.464	-972.290	62.593	14.077	284.874
ALOH	43.98888	-203.114	-190.000	-192.762	43.512	10.352	222.643
ALOHCL	79.44158	-387.705	-370.000	-373.786	57.901	13.919	294.387
ALOHCL2	114.89428	-742.295	-720.000	-725.145	77.819	17.150	325.075
ALOHF	62.98728	-587.527	-570.000	-574.212	54.626	13.315	282.240
ALOHF2	81.98568	-1156.939	-1135.000	-1141.511	70.799	15.428	299.541
ALO2	58.98034	-52.020	-38.799	-38.658	51.661	13.362	269.317
ALO2-	58.98089	-463.217	-443.799	-452.572	46.063	10.645	229.783
AL(OH) 2	60.99622	-521.688	-500.000	-507.661	62.980	14.028	284.406
AL(OH) 2CL	96.44892	-876.279	-850.000	-859.057	82.994	17.222	316.305
AL(OH) 2F	79.99462	-1086.101	-1060.000	-1069.629	79.532	16.472	304.655
AL(OH) 3	78.00356	-1030.262	-1000.000	-1012.668	87.249	17.595	301.541
ALS	59.04754	223.594	232.546	232.682	33.405	9.088	230.619
ALS2	91.11354	234.107	247.471	248.535	56.557	14.429	294.462
AL2	53.96308	491.163	500.243	501.302	37.055	10.139	243.842
AL2Br6	533.38708	-980.640	-898.000	-942.423	167.510	38.217	537.155
AL2C2	77.98448	528.813	540.000	544.978	67.665	16.165	284.603
AL2CL6	266.67928	-1331.023	-1294.400	-1296.876	159.150	34.147	470.448
AL2F6	167.95350	-2658.555	-2623.000	-2632.491	133.312	26.064	385.487
AL2I6	815.38990	-528.668	-480.000	-487.747	171.922	40.921	589.636
AL2O	69.96248	-161.388	-147.968	-148.611	51.978	12.777	253.135
AL2O+	69.96193	635.989	643.212	648.970	52.898	12.981	260.663
AL2O2	85.96188	-418.938	-401.178	-403.096	68.122	15.843	288.044
AL2O2+	85.96133	542.464	554.026	557.439	68.924	14.975	289.704
AL2O3	101.96128	-566.489	-544.388	-546.891	86.990	19.598	316.662
AL2S	86.02908	206.675	220.167	220.679	56.379	14.004	271.338
AL2S2	118.09508	117.188	135.092	135.287	75.938	18.100	320.299
Ar	39.94800	-6.197	-6.197	0.000	20.786	6.197	154.847
Ar+	39.94745	1520.572	1520.572	1526.778	20.984	6.206	166.406
B	10.81100	569.283	570.497	575.599	20.797	6.316	153.438
B+	10.81045	1376.118	1371.135	1382.316	20.786	6.197	138.545
B-	10.81155	536.359	543.770	542.631	20.788	6.273	156.814
BBr	90.71500	231.955	245.429	240.952	32.787	8.997	224.992
BBr2	170.61900	85.628	111.362	97.829	48.451	12.201	294.539
BBr3	250.52300	-221.003	-183.009	-205.300	67.777	15.703	324.505
BC	22.82170	829.427	831.694	838.162	30.217	8.735	210.103
BC2	34.83240	789.571	792.892	801.259	45.718	11.688	236.684
BCL	46.26370	174.312	180.117	183.173	31.656	8.861	213.244
BCL+	46.26315	1225.420	1225.027	1234.280	31.644	8.860	219.133
BCLOH	63.27104	-246.437	-232.058	-234.005	52.322	12.432	272.255
BCL(OH) 2	80.27838	-818.953	-796.000	-805.388	68.307	13.565	285.524
BCL2	81.71640	-72.395	-62.000	-60.881	45.746	11.514	271.202
BCL2+	81.71585	659.467	663.664	672.315	52.975	12.849	257.809
BCL2OH	98.72374	-618.969	-600.000	-604.917	66.824	14.052	296.758

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
BCL3	117.16910	-418.471	-403.485	-404.500	62.556	13.971	289.468
BF	29.80940	-115.627	-110.000	-106.932	29.594	8.695	200.453
BFCL	65.26210	-290.217	-280.000	-279.184	42.820	11.033	264.941
BFCL2	100.71480	-656.231	-641.423	-643.000	58.911	13.231	287.581
BFOH	46.81674	-463.605	-449.404	-451.632	49.233	11.973	260.090
BF(OH) 2	63.82408	-1062.775	-1040.000	-1049.890	63.510	12.885	274.274
BF2	48.80781	-510.039	-500.000	-499.427	40.055	10.612	247.133
BF2+	48.80726	311.974	315.816	322.586	44.291	10.612	225.151
BF2-	48.80835	-744.237	-728.000	-733.803	39.436	10.434	240.589
BF2CL	84.26051	-900.324	-885.694	-888.000	54.473	12.324	275.115
BF2OH	65.81515	-1104.613	-1086.000	-1092.217	57.769	12.396	272.590
BF3	67.80621	-1147.651	-1133.200	-1136.000	50.462	11.651	254.429
BF4-	86.80516	-1775.062	-1750.000	-1761.266	67.794	13.796	268.855
BH	11.81894	440.088	445.536	448.727	29.181	8.639	171.836
BHCL	47.27164	131.113	141.152	141.418	38.435	10.305	240.471
BHCL2	82.72434	-263.629	-249.000	-251.884	49.656	11.746	268.244
BHF	30.81734	-86.054	-76.194	-76.012	35.458	10.042	227.969
BHFCL	66.27004	-494.451	-480.000	-483.037	47.771	11.415	263.145
BHF2	49.81575	-750.273	-736.000	-739.614	42.230	10.659	244.323
BH2	12.82688	318.885	328.568	328.909	34.975	10.024	193.685
BH2CL	48.27958	-91.273	-77.000	-80.846	40.345	10.427	234.358
BH2F	31.82528	-334.095	-320.000	-323.957	37.204	10.138	222.022
BH3	13.83482	94.687	108.603	104.747	36.018	10.060	188.251
BH3NH3	30.86538	-127.682	-96.728	-115.000	56.999	12.682	240.883
BH4	14.84276	244.440	262.590	255.210	44.277	10.771	211.994
BH5	15.85070	80.361	102.745	92.934	52.616	12.572	229.549
BI	137.71547	316.845	324.657	325.988	33.731	9.142	233.319
BI2	264.61994	225.408	239.818	238.096	50.294	12.688	311.115
BI3	391.52441	4.467	25.475	21.400	71.027	16.933	350.427
BN	24.81774	565.765	571.314	574.726	29.519	8.961	212.781
BO	26.81040	11.732	17.286	20.406	29.196	8.674	203.468
BO-	26.81095	-286.465	-274.714	-277.791	29.197	8.674	197.683
BOCL	62.26310	-329.145	-319.000	-318.537	45.079	10.608	237.306
BOCL2	97.71580	-374.735	-360.000	-361.566	58.826	13.170	292.296
BOF	45.80880	-602.967	-593.000	-592.978	41.653	9.988	224.981
BOF2	64.80721	-844.379	-830.000	-832.768	50.491	11.611	268.239
BOH	27.81834	-16.788	-7.000	-6.757	35.350	10.032	217.899
BO2	42.80980	-319.894	-310.000	-309.122	43.285	10.772	230.138
BO2-	42.81035	-724.092	-708.000	-714.494	39.147	9.598	215.734
B(OH) 2	44.82568	-437.215	-418.853	-425.244	54.191	11.972	259.389
BS	42.87700	264.795	270.421	273.519	30.052	8.724	216.195
BS2	74.94300	50.308	60.346	63.867	55.498	13.560	267.139
B2	21.62200	848.565	850.993	857.371	31.503	8.805	202.064
B2C	33.63270	788.710	792.191	800.433	46.228	11.723	225.242
B2CL4	163.43280	-511.588	-490.798	-490.000	97.997	21.588	371.268
B2F4	97.61561	-1455.681	-1435.603	-1438.000	80.629	17.681	326.206
B2H	22.62994	786.147	792.809	796.262	42.328	10.116	214.282
B2H2	23.63788	444.105	455.001	454.678	48.195	10.573	214.235
B2H3	24.64582	339.134	354.264	351.073	52.523	11.939	236.055
B2H3, db	24.64582	341.497	356.627	353.408	52.473	11.911	232.835
B2H4	25.65376	198.822	218.186	211.162	57.117	12.340	230.385
B2H4, db	25.65376	198.404	217.768	209.932	51.510	11.529	228.028
B2H5	26.66170	242.563	266.161	254.784	58.182	12.221	243.502
B2H5, db	26.66170	263.483	287.081	275.151	53.171	11.668	245.703
B2H6	27.66964	24.668	52.500	36.600	56.643	11.932	232.027

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
B2O	37.62140	181.015	187.783	192.798	47.247	11.783	226.244
B2O2	53.62080	-471.108	-460.000	-457.711	60.269	13.397	249.669
B2O3	69.62020	-849.801	-834.353	-835.382	64.917	14.419	285.902
B2 (OH) 4	89.65136	-1274.431	-1237.706	-1254.988	105.026	19.443	347.137
B2S	53.68800	609.078	615.918	622.261	52.763	13.183	248.243
B2S2	85.75400	123.748	135.000	138.317	65.492	14.569	271.346
B2S3	117.82000	-2.184	13.480	17.754	82.668	19.938	351.434
B3H7, C2v	39.48858	161.201	194.481	176.019	81.606	14.818	265.948
B3H7, Cs	39.48858	145.235	178.515	159.318	76.693	14.083	267.986
B3H9	41.50446	121.579	163.327	138.909	95.357	17.330	282.497
B3N3H6	80.50086	-528.221	-486.170	-512.000	93.888	16.221	287.642
B3O3CL3	186.78930	-1660.434	-1630.000	-1635.982	124.123	24.452	380.039
B3O3FCL2	170.33500	-1907.256	-1877.000	-1883.808	120.642	23.448	377.597
B3O3F2CL	153.88071	-2155.078	-2125.000	-2132.817	115.328	22.261	364.875
B3O3F3	137.42641	-2403.900	-2374.000	-2382.699	110.653	21.201	343.946
B4H4	47.27576	311.254	333.046	326.190	80.417	14.937	277.068
B4H10	53.32340	50.614	97.811	66.100	93.147	15.486	280.152
B4H12	55.33928	166.487	222.152	188.236	128.224	21.749	315.870
B5H9	63.12646	57.167	101.344	73.220	99.564	16.053	280.603
Ba	137.32700	178.803	185.710	185.000	20.786	6.197	170.247
Ba+	137.32645	687.852	688.562	694.050	20.786	6.197	176.010
BaBr	217.23100	-85.525	-66.358	-75.325	37.002	10.200	270.851
BaBr2	297.13500	-428.000	-396.574	-412.515	57.359	15.486	347.959
BaCL	172.77970	-146.168	-134.670	-136.291	36.440	9.877	258.839
BaCL+	172.77915	339.029	344.330	348.698	35.874	9.668	251.733
BaCL2	208.23240	-513.900	-497.812	-499.301	56.113	14.599	323.490
BaF	156.32540	-328.336	-317.016	-318.994	34.747	9.342	246.214
BaF+	156.32485	124.862	129.984	134.063	34.046	9.202	239.222
BaF2	175.32381	-825.441	-809.708	-812.003	53.272	13.437	298.673
BaH	138.33494	200.804	211.945	209.535	30.232	8.731	219.009
BaI	264.23147	-20.635	-7.130	-10.238	37.315	10.397	278.578
BaI2	391.13594	-304.230	-284.127	-288.440	57.632	15.790	361.977
BaO	153.32640	-126.963	-115.715	-117.948	32.898	9.014	235.460
BaO+	153.32585	502.235	507.285	511.705	37.467	9.470	244.661
BaOH	154.33434	-235.481	-220.000	-224.257	47.723	11.225	255.755
BaOH+	154.33379	190.716	200.000	202.019	48.054	11.303	251.098
Ba (OH) 2	171.34168	-624.055	-600.000	-606.666	79.954	17.389	318.658
BaS	169.39300	29.315	40.634	38.871	35.532	9.556	248.864
Ba2	274.65400	344.605	358.419	355.964	37.016	11.359	290.710
Be	9.01218	317.803	319.745	324.000	20.786	6.197	136.276
Be+	9.01163	1223.504	1219.249	1229.701	20.786	6.197	142.039
Be++	9.01108	2986.804	2976.351	2993.002	20.786	6.197	136.275
BeBr	88.91618	123.475	137.677	132.446	32.598	8.971	229.591
BeBr2	168.82018	-246.900	-220.438	-234.062	53.252	12.838	273.241
BeCL	44.46488	47.832	54.365	56.693	31.650	8.861	218.100
BeCL2	79.91758	-373.620	-362.497	-361.539	51.048	12.081	250.263
BeF	28.01059	-179.336	-172.981	-170.625	29.872	8.711	205.754
BeF2	47.00899	-807.468	-796.701	-796.588	45.884	10.880	227.283
BeH	10.02012	333.604	339.780	342.252	29.224	8.648	176.823
BeH+	10.01957	1169.575	1169.554	1178.219	29.193	8.644	170.655
BeH2	11.02806	151.880	162.290	161.099	35.843	9.219	175.235
BeI	135.91665	198.365	206.905	207.454	33.401	9.089	237.579
BeI2	262.82112	-78.200	-63.062	-64.759	54.719	13.441	289.396
BeN	23.01892	418.275	424.552	427.000	30.089	8.725	208.770
BeO	25.01158	120.252	126.534	128.940	29.479	8.688	197.604

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
BeOH	26.01952	-110.516	-100.000	-99.718	43.642	10.798	217.058
BeOH+	26.01897	750.433	754.752	759.984	38.441	9.551	203.922
Be (OH) 2	43.02686	-654.090	-635.000	-638.864	74.066	15.226	249.019
BeS	41.07818	238.315	244.669	247.095	30.786	8.780	210.286
Be2	18.02436	627.705	631.589	637.543	30.667	9.838	203.724
Be2CL4	159.83516	-842.246	-820.000	-819.605	105.515	22.641	366.340
Be2F4	94.01798	-1751.534	-1730.000	-1731.700	94.916	19.835	323.167
Be2O	34.02376	-48.224	-40.000	-37.034	47.783	11.190	227.956
Be2OF2	72.02057	-1221.159	-1204.110	-1204.574	76.152	16.585	298.919
Be2O2	50.02316	-422.564	-410.000	-411.635	46.287	10.929	243.042
Be3O3	75.03475	-1038.846	-1020.000	-1023.721	75.946	15.126	283.180
Be4O4	100.04633	-1665.128	-1640.000	-1649.295	88.657	15.834	296.472
Br	79.90400	105.673	117.933	111.870	20.786	6.197	175.019
Br+	79.90345	1251.730	1257.792	1257.927	20.787	6.197	176.874
Br-	79.90455	-225.198	-206.740	-219.000	20.786	6.197	163.493
BrCL	115.35670	5.382	22.233	14.789	35.011	9.407	240.049
BrF	98.90240	-67.873	-51.200	-58.851	32.959	9.021	228.988
BrF3	136.89921	-270.312	-244.814	-255.600	67.354	14.712	295.775
BrF5	174.89602	-447.975	-413.652	-428.800	101.335	19.175	323.253
BrO	95.90340	116.739	133.339	125.800	34.182	9.061	232.970
OBRO	111.90280	140.560	161.500	151.955	45.364	11.395	271.112
BrOO	111.90280	95.149	116.089	108.000	48.875	12.851	288.845
BrO3	127.90220	207.720	233.000	220.821	59.999	13.101	284.509
Br2	159.80800	21.185	45.705	30.910	36.057	9.725	245.469
BrBrO	175.80740	154.863	183.723	168.000	51.385	13.137	312.704
BrOBr	175.80740	95.240	124.100	107.639	50.168	12.399	290.823
C	12.01070	710.144	711.198	716.680	20.839	6.536	158.101
C+	12.01015	1802.795	1797.651	1809.444	20.974	6.649	154.663
C-	12.01125	582.095	589.346	588.314	20.787	6.219	159.003
CBr	91.91470	480.817	494.130	490.432	35.534	9.615	234.562
CBr2	171.81870	324.426	350.000	336.623	49.304	12.197	288.465
CBr3	251.72270	219.418	257.251	235.000	67.440	15.582	334.577
CBr4	331.62670	59.127	109.220	79.500	91.138	20.373	357.954
CCL	47.46340	423.216	428.860	432.611	32.268	9.395	224.556
CCLBr3	287.17540	45.432	87.856	65.000	89.299	19.568	357.617
CCL2	82.91610	211.517	221.752	222.940	46.305	11.423	264.872
CCL2Br2	242.72410	-8.692	26.063	10.000	87.053	18.692	348.490
CCL3	118.36880	56.728	71.553	71.128	63.500	14.400	303.100
CCL3Br	198.27280	-60.985	-33.899	-43.000	85.204	17.985	333.580
CCL4	153.82150	-112.759	-93.343	-95.600	82.890	17.159	309.467
CF	31.00910	233.235	238.701	242.300	30.056	9.065	213.034
CF+	31.00855	1136.867	1136.135	1145.564	29.642	8.697	201.509
CFBr3	270.72110	-138.243	-95.997	-120.000	84.257	18.243	345.725
CFCL	66.46180	14.943	25.000	25.846	42.962	10.902	259.150
CFCLBr2	226.26980	-192.498	-157.921	-175.000	82.338	17.498	343.087
CFCL2	101.91450	-118.217	-103.570	-105.000	59.121	13.217	298.917
CFCL2Br	181.81850	-251.731	-224.823	-235.000	80.108	16.731	330.773
CFCL3	137.36720	-299.764	-280.526	-283.700	78.071	16.064	309.785
CF2	50.00751	-196.951	-187.072	-186.600	38.915	10.351	240.831
CF2+	50.00696	938.999	942.680	949.341	38.541	10.342	246.731
CF2Br2	209.81551	-396.280	-361.881	-380.000	77.000	16.280	325.413
CF2CL	85.46021	-287.432	-272.963	-275.000	55.172	12.432	287.353
CF2CLBr	165.36421	-450.528	-423.799	-435.000	74.650	15.528	318.724
CF2CL2	120.91291	-505.681	-486.621	-490.800	72.477	14.881	300.908
CF3	69.00591	-478.891	-464.600	-467.400	49.642	11.491	264.521

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
CF3+	69.00536	412.076	420.170	423.617	49.339	11.541	254.540
CF3Br	148.90991	-663.244	-636.693	-648.800	69.270	14.444	297.695
CF3CL	104.45861	-717.991	-699.109	-704.200	66.887	13.791	285.424
CF4	88.00431	-945.850	-927.147	-933.120	61.052	12.730	261.459
CH	13.01864	588.745	594.033	597.371	29.175	8.625	183.040
CH+	13.01809	1621.943	1621.033	1630.571	29.154	8.628	171.673
CHBr3	252.73064	0.833	42.901	16.740	70.982	15.907	330.705
CHCL	48.47134	286.900	296.778	297.100	37.787	10.200	235.062
CHCLBr2	208.27934	-5.291	29.107	10.000	69.149	15.291	328.026
CHCL2	83.92404	83.000	97.469	95.800	53.900	12.800	285.500
CHCL2Br	163.82804	-59.730	-33.001	-45.000	67.395	14.730	316.478
CHCL3	119.37674	-117.005	-97.946	-102.700	66.879	14.305	296.374
CHF	32.01704	98.819	108.519	108.800	34.588	9.981	223.342
CHBr2	191.82504	-189.360	-155.139	-175.000	64.915	14.360	316.925
CHFCL	67.46974	-94.291	-80.000	-83.145	45.077	11.146	268.507
CHFCLBr	147.37374	-243.787	-217.237	-230.000	62.869	13.787	310.691
CHFCL2	102.92244	-298.194	-279.313	-284.900	61.010	13.294	293.308
CHF2	51.01545	-249.820	-235.707	-238.900	43.062	10.920	258.000
CHF2Br	130.91945	-435.170	-408.797	-422.000	58.767	13.170	295.230
CHF3	70.01385	-704.867	-686.342	-693.300	51.082	11.567	259.689
CHI3	393.73205	193.717	218.799	210.874	75.072	17.157	355.622
CH2	14.02658	380.337	389.859	390.365	35.015	10.027	194.419
CH2Br2	173.83458	-27.384	6.657	-14.770	54.552	12.614	293.391
CH2CL	49.47958	108.220	122.332	119.200	43.173	10.980	242.634
CH2CLBr	129.38358	-57.191	-30.819	-45.000	52.726	12.191	287.290
CH2CL2	84.93258	-106.854	-88.151	-95.000	50.951	11.854	270.365
CH2F	33.02498	-42.929	-28.995	-31.800	42.442	11.129	233.700
CH2FBr	112.92898	-226.623	-200.428	-215.000	49.089	11.623	276.282
CH2FCL	68.47798	-276.952	-258.428	-265.700	47.046	11.252	264.426
CH2F2	52.02339	-462.993	-444.647	-452.300	42.880	10.693	246.711
CH2I2	267.83552	104.320	127.038	117.570	57.735	13.250	309.504
CH3	15.03452	136.292	150.047	146.658	38.417	10.366	194.009
CH3Br	94.93852	-48.353	-22.337	-37.740	42.455	10.613	245.959
CH3CL	50.48752	-92.286	-73.940	-81.870	40.741	10.416	234.396
CH3F	34.03292	-247.835	-229.667	-237.700	37.504	10.135	222.826
CH3I	141.93899	2.950	23.303	13.765	44.084	10.816	253.807
CH2OH	31.03392	-29.581	-11.485	-17.800	47.401	11.781	244.170
CH2OH+	31.03337	706.251	718.149	716.400	37.835	10.149	228.047
CH3O	31.03392	1.698	19.794	13.000	47.012	11.302	236.066
CH4	16.04246	-84.616	-66.626	-74.600	35.691	10.016	186.371
CH3OH	32.04186	-212.375	-190.046	-200.940	44.039	11.435	239.810
CH3OOH	48.04126	-152.919	-126.249	-139.000	61.690	13.919	276.504
CI	138.91517	560.707	568.358	570.201	36.908	9.494	241.318
CI2	265.81964	455.750	470.000	468.394	50.945	12.643	304.324
CI3	392.72411	389.152	410.000	405.984	70.550	16.831	361.033
CI4	519.62858	245.588	273.033	267.943	95.842	22.356	391.740
CN	26.01740	430.011	435.400	438.684	29.156	8.672	202.646
CN+	26.01685	1790.209	1789.400	1798.891	29.463	8.682	196.935
CN-	26.01795	55.214	66.800	63.885	29.151	8.671	196.576
CNN	40.02410	623.106	632.830	633.484	42.656	10.378	232.398
CO	28.01010	-119.206	-113.813	-110.535	29.141	8.671	197.660
CO+	28.00955	1239.118	1238.314	1247.789	29.137	8.671	203.230
COCL	63.46310	-27.551	-17.567	-16.000	45.073	11.551	265.195
COCL2	98.91610	-232.379	-217.804	-219.500	57.761	12.879	283.752

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
COFCL	82.46150	-441.397	-427.000	-429.493	52.397	11.904	276.705
COF2	66.00691	-651.134	-636.915	-640.000	47.365	11.134	258.971
COHCL	64.47104	-175.218	-161.000	-164.212	44.679	11.006	259.070
COHF	48.01644	-385.040	-371.000	-374.590	40.502	10.450	246.828
COS	60.07510	-151.642	-141.836	-141.700	41.549	9.942	231.650
CO2	44.00950	-402.875	-393.142	-393.510	37.135	9.365	213.787
CO2+	44.00895	934.122	937.658	944.688	41.799	10.566	228.017
COOH	45.01744	-223.813	-209.846	-213.000	43.610	10.813	251.736
CP	42.98446	511.447	517.860	520.162	29.910	8.715	216.257
CS	44.07570	269.842	275.307	278.550	29.799	8.708	210.558
CS2	76.14070	106.036	115.913	116.700	45.482	10.664	237.889
C2	24.02140	820.288	822.395	830.457	43.549	10.169	197.097
C2+	24.02085	1996.090	1992.000	2004.776	29.400	8.685	204.179
C2-	24.02195	472.091	480.395	480.767	29.241	8.676	196.599
C2CL	59.47440	523.302	530.000	534.083	45.046	10.781	241.948
C2CL2	94.92740	212.007	223.296	226.600	65.374	14.593	272.112
C2CL3	130.38040	174.121	190.000	190.272	76.033	16.150	328.166
C2CL4	165.83340	-43.806	-23.336	-24.200	94.920	19.606	341.034
C2CL6	236.73940	-175.329	-145.679	-148.200	136.348	27.129	398.632
C2F	43.01980	343.480	350.000	353.847	42.600	10.367	231.036
C2FCL	78.47280	19.890	31.000	33.766	62.627	13.877	266.386
C2FCL3	149.37880	-184.732	-164.441	-166.000	91.032	18.732	342.594
C2F2	62.01821	-157.932	-147.000	-144.666	60.114	13.266	249.570
C2F2CL2	132.92421	-355.773	-335.660	-337.837	89.506	17.936	326.491
C2F3	81.01661	-242.345	-227.000	-228.181	66.178	14.164	297.643
C2F3CL	116.46961	-532.328	-512.393	-515.200	83.917	17.128	322.389
C2F4	100.01501	-675.831	-656.073	-659.500	80.459	16.331	300.128
C2F6	138.01182	-1364.272	-1335.690	-1344.000	106.211	20.272	332.434
C2H	25.02934	555.752	562.093	566.200	42.000	10.449	213.304
C2HCL	60.48234	214.612	225.544	226.400	54.320	11.788	241.955
C2HCL3	131.38834	-34.105	-13.992	-17.500	80.016	16.605	324.942
C2HF	44.02774	30.246	41.000	41.692	52.268	11.446	231.573
C2HFCL2	114.93374	-184.907	-164.973	-168.648	77.324	16.259	320.191
C2HF2CL	98.47915	-348.917	-329.160	-333.654	76.650	15.263	304.242
C2HF3	82.02455	-505.328	-485.749	-491.000	69.191	14.328	292.665
C2H2, acetylene	26.03728	218.194	228.769	228.200	44.001	10.006	200.916
C2H2, vinylidene	26.03728	403.914	414.489	414.788	42.614	10.874	221.021
C2H2CL2	96.94328	-11.472	8.284	3.410	68.847	14.882	297.021
C2H2FCL	80.48868	-178.551	-158.973	-165.082	68.337	13.469	284.542
C2H2F2	64.03409	-348.880	-329.479	-336.400	60.237	12.480	266.054
CH2CO, ketene	42.03668	-61.372	-46.457	-49.576	51.740	11.796	251.442
O (CH) 2O	58.03608	-225.682	-206.427	-212.000	60.409	13.682	272.483
HO (CO) 2OH	90.03488	-749.122	-721.186	-731.800	86.178	17.322	320.649
C2H3, vinyl	27.04522	289.165	303.974	299.687	42.071	10.522	233.663
CH2Br-COOH	138.94802	-400.362	-364.613	-383.500	80.542	16.862	337.015
C2H3CL	62.49822	10.180	29.580	22.000	53.681	11.820	264.024
CH2CL-COOH	94.49672	-444.114	-416.034	-427.600	78.839	16.514	325.918
C2H3F	46.04362	-151.436	-132.214	-140.100	50.407	11.336	252.674
CH3CN	41.05192	54.336	73.481	66.430	52.246	12.094	243.460
CH3CO, acetyl	43.04462	-23.036	-3.887	-10.000	54.642	13.036	270.320
C2H4	28.05316	41.981	61.025	52.500	42.887	10.519	219.322
C2H4O, ethylen-o	44.05256	-63.465	-40.082	-52.635	47.624	10.831	242.870
CH3CHO, ethanal	44.05256	-179.087	-155.703	-166.190	55.319	12.897	263.952
CH3COOH	60.05196	-445.846	-418.123	-432.249	63.439	13.597	283.473
OHCH2COOH	76.05136	-600.007	-567.944	-583.000	87.076	17.007	318.614

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
C2H5	29.06110	106.473	129.750	118.658	50.484	12.185	247.118
C2H5Br	108.96510	-77.169	-41.632	-63.600	64.230	13.569	287.250
C2H6	30.06904	-95.743	-68.232	-83.852	52.501	11.892	229.221
CH3N2CH3	58.08244	132.174	168.356	148.699	78.063	16.525	289.823
C2H5OH	46.06844	-249.492	-217.641	-234.950	65.309	14.542	280.593
CH3OCH3	46.06844	-198.464	-166.613	-184.110	65.823	14.354	267.381
CH3O2CH3	62.06784	-142.653	-106.462	-125.500	80.719	17.153	308.414
CCN	38.02810	793.558	800.000	804.596	44.231	11.039	237.159
CNC	38.02810	673.558	680.000	684.915	45.042	11.357	233.804
OCCN	54.02754	196.406	207.188	210.000	56.145	13.594	278.187
C2N2	52.03480	296.385	307.162	309.100	57.085	12.715	242.204
C2O	40.02080	280.553	287.000	291.039	43.134	10.486	233.624
C2S2	88.15140	362.900	373.831	376.660	62.030	13.760	274.120
C3	36.03210	827.840	831.000	839.949	42.203	12.109	237.613
C3H3,1-propynl	39.05592	437.600	453.463	450.000	53.000	12.400	250.900
C3H3,2-propynl	39.05592	318.570	334.433	331.800	62.640	13.230	254.520
C3H4,allene	40.06386	178.315	198.412	190.920	58.880	12.605	243.630
C3H4,propyne	40.06386	171.869	191.966	184.900	60.731	13.031	248.428
C3H4,cyclo-	40.06386	265.726	285.823	277.100	52.883	11.374	243.605
C3H5,allyl	41.07180	150.856	175.186	163.594	63.387	12.739	258.886
C3H6,propylene	42.07974	6.449	35.014	20.000	64.433	13.551	266.668
C3H6,cyclo-	42.07974	41.890	70.455	53.300	55.572	11.410	237.488
C3H6O,propylox	58.07914	-108.125	-75.221	-93.720	72.370	14.405	281.523
C3H6O,acetone	58.07914	-233.343	-200.438	-217.150	74.207	16.193	295.660
C3H6O,propanal	58.07914	-203.327	-170.422	-186.000	84.472	17.327	300.873
C3H7,n-propyl	43.08768	85.640	118.439	100.500	71.211	14.860	289.586
C3H7,i-propyl	43.08768	78.493	111.292	93.300	66.314	14.807	289.494
C3H8	44.09562	-119.421	-82.388	-104.680	73.589	14.741	270.315
C3H8O,1propanol	60.09502	-272.719	-231.346	-255.200	84.978	17.519	323.367
C3H8O,2propanol	60.09502	-289.965	-248.592	-272.700	89.596	17.265	309.226
CNCOCN	80.04498	230.352	246.523	247.500	80.854	17.148	310.032
C3OS	84.09650	141.610	153.523	157.330	72.150	15.720	289.180
C3O2	68.03090	-108.723	-96.882	-93.638	67.370	15.085	276.816
C3S2	100.16210	396.510	408.494	412.500	74.780	15.990	288.340
C4	48.04280	1020.786	1025.000	1033.904	57.272	13.118	252.861
C4H2,butadiyne	50.05868	435.606	448.288	450.000	73.675	14.394	250.251
C4H4,1,3-cyclo-	52.07456	372.896	394.047	385.000	60.969	12.104	251.442
C4H6,butadiene	54.09044	94.870	124.488	110.000	79.810	15.130	278.780
C4H6,1butyne	54.09044	149.180	178.798	165.200	81.820	16.020	291.210
C4H6,2butyne	54.09044	129.060	158.678	145.700	78.020	16.640	284.210
C4H6,cyclo-	54.09044	144.142	173.761	156.700	64.414	12.558	262.076
C4H8,1-butene	56.10632	-17.660	20.426	-0.540	85.560	17.120	307.860
C4H8,cis2-buten	56.10632	-24.200	13.886	-7.400	80.150	16.800	301.310
C4H8,tr2-butene	56.10632	-28.510	9.576	-11.000	87.670	17.510	296.330
C4H8,isobutene	56.10632	-34.110	3.976	-17.100	88.090	17.010	293.200
C4H8,cyclo-	56.10632	14.866	52.952	28.400	70.565	13.534	264.509
(CH3COOH)2	120.10392	-957.069	-901.622	-929.015	137.254	28.053	414.396
C4H9,n-butyl	57.11426	46.733	89.053	66.530	97.670	19.797	328.519
C4H9,i-butyl	57.11426	39.003	81.323	57.320	95.530	18.317	318.649
C4H9,s-butyl	57.11426	53.462	95.783	71.000	87.392	17.538	334.126
C4H9,t-butyl	57.11426	34.690	77.011	51.700	78.225	17.010	319.719
C4H10,n-butane	58.12220	-145.019	-98.464	-125.790	98.657	19.229	309.881
C4H10,isobutane	58.12220	-152.927	-106.372	-134.990	96.643	17.936	295.493
C4N2	76.05620	511.401	524.285	529.200	86.326	17.799	290.524
C5	60.05350	1034.733	1040.000	1050.924	75.507	16.192	271.677



# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
C5H6,1,3cyclo-	66.10114	120.764	151.436	134.300	75.369	13.536	274.154
C5H8,cyclo-	68.11702	19.043	58.183	33.900	81.276	14.857	291.380
C5H10,1-pentene	70.13290	-42.960	4.648	-21.280	108.200	21.680	347.110
C5H10,cyclo-	70.13290	-92.123	-44.515	-77.100	82.761	15.023	293.009
C5H11,pentyl	71.14084	21.388	73.230	45.810	119.150	24.422	368.649
C5H11,t-pentyl	71.14084	12.956	64.798	32.600	98.856	19.644	366.476
C5H12,n-pentane	72.14878	-170.944	-114.868	-146.760	120.040	24.184	349.560
C5H12,i-pentane	72.14878	-175.708	-119.632	-153.700	118.870	22.008	343.740
CH3C(CH3)2CH3	72.14878	-191.099	-135.023	-167.920	120.830	23.179	306.000
C6D5,phenyl	82.13471	299.821	327.565	315.740	94.997	15.919	300.504
C6D6	84.14881	41.833	73.861	58.157	100.398	16.325	282.629
C6H2	74.08008	650.392	665.181	670.000	103.919	19.608	298.911
C6H5,phenyl	77.10390	323.045	350.537	337.200	80.583	14.155	288.868
C6H5O,phenoxy	93.10330	31.492	63.323	47.700	94.143	16.208	307.896
C6H6	78.11184	68.684	100.410	82.880	81.935	14.196	269.159
C6H5OH,phenol	94.11124	-113.896	-77.830	-96.399	103.339	17.497	315.240
C6H10,cyclo-	82.14360	-21.871	26.791	-4.600	101.464	17.271	310.633
C6H12,1-hexene	84.15948	-68.190	-11.060	-41.950	130.800	26.240	386.350
C6H12,cyclo-	84.15948	-140.845	-83.715	-123.300	105.344	17.545	297.391
C6H13,n-hexyl	85.16742	-3.883	57.481	25.100	141.790	28.983	408.339
C6H14,n-hexane	86.17536	-195.622	-130.024	-166.920	142.590	28.702	388.850
C7H7,benzyl	91.13048	191.945	228.958	210.500	109.126	18.555	321.133
C7H8	92.13842	32.230	73.477	50.170	103.280	17.940	320.188
C7H8O,cresol-mx	108.13782	-154.136	-108.549	-132.298	128.027	21.838	360.118
C7H14,1-heptene	98.18606	-93.550	-26.899	-62.760	153.500	30.790	425.600
C7H15,n-heptyl	99.19400	-29.153	41.732	4.390	164.430	33.543	448.029
C7H16,n-heptane	100.20194	-221.001	-145.882	-187.780	165.180	33.221	428.089
C7H16,2-methylh	100.20194	-225.520	-150.401	-194.600	164.500	30.920	420.500
C8H8,styrene	104.14912	127.360	169.660	148.300	120.190	20.940	344.770
C8H10,ethylbenz	106.16500	7.640	58.409	29.920	127.400	22.280	360.630
C8H16,1-octene	112.21264	-118.940	-42.767	-83.590	176.100	35.350	464.840
C8H17,n-octyl	113.22058	-54.423	25.984	-16.320	187.070	38.103	487.729
C8H18,n-octane	114.22852	-246.530	-161.889	-208.750	187.780	37.780	467.350
C8H18,isooctane	114.22852	-256.180	-171.539	-224.010	188.410	32.170	423.090
C9H19,n-nonyl	127.24716	-79.694	10.234	-37.030	209.710	42.664	527.419
C10H8,naphthale	128.17052	129.867	174.274	150.580	131.920	20.713	333.267
C10H21,n-decyl	141.27374	-104.964	-5.514	-57.740	232.350	47.224	567.109
C12H9,o-bipheny	153.19986	401.141	451.889	427.730	163.049	26.589	405.113
C12H10,biphenyl	154.20780	155.346	210.329	182.130	166.179	26.784	388.944
Ca	40.07800	171.603	177.386	177.800	20.786	6.197	154.887
Ca+	40.07745	767.630	767.216	773.828	20.786	6.197	160.650
CaBr	119.98200	-34.725	-16.682	-24.869	36.390	9.856	253.125
CaBr2	199.88600	-402.800	-372.498	-387.197	60.287	15.603	310.134
CaCL	75.53100	-113.368	-102.995	-103.773	35.686	9.595	241.635
CaCL+	75.53045	457.829	462.005	467.191	34.811	9.361	233.154
CaCL2	110.98400	-500.101	-485.136	-485.243	59.050	14.857	286.396
CaF	59.07640	-285.536	-275.340	-276.404	33.671	9.132	229.138
CaF+	59.07585	251.661	255.660	260.665	32.824	9.003	222.299
CaF2	78.07481	-803.640	-789.032	-790.828	51.208	12.812	274.396
CaH	41.08594	220.704	230.721	229.409	29.896	8.705	201.844
CaI	166.98247	2.165	14.546	12.183	36.708	10.018	261.058
CaI2	293.88694	-275.370	-256.392	-259.320	60.835	16.051	326.578
CaO	56.07740	29.052	39.175	38.005	32.454	8.953	219.719
CaO+	56.07685	701.074	705.000	710.238	34.537	9.163	233.606
CaOH	57.08534	-184.357	-170.000	-173.307	46.733	11.050	238.853

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
CaOH+	57.08479	361.840	370.000	372.938	47.039	11.098	233.924
Ca (OH) 2	74.09268	-614.931	-592.000	-598.339	77.001	16.592	292.045
CaS	72.14300	112.115	122.310	121.475	34.813	9.360	232.617
Ca2	80.15600	330.492	342.058	341.765	36.995	11.273	257.567
Cd	112.41100	105.603	111.850	111.800	20.786	6.197	167.750
Cd+	112.41045	979.557	979.606	985.754	20.786	6.197	173.513
CL	35.45300	115.029	119.620	121.301	21.838	6.272	165.192
CL+	35.45245	1372.413	1370.806	1378.800	22.959	6.386	167.558
CL-	35.45355	-240.155	-229.367	-233.958	20.786	6.197	153.358
CLCN	61.47040	123.531	133.510	134.200	44.960	10.669	236.144
CLF	54.45140	-64.609	-55.606	-55.701	32.085	8.908	217.943
CLF3	92.44821	-178.328	-160.500	-164.600	64.061	13.728	282.152
CLF5	130.44502	-255.930	-229.277	-238.000	97.167	17.930	310.257
CLO	51.45240	92.099	101.030	101.621	34.471	9.522	225.104
CLO2	67.45180	94.199	107.470	105.000	42.004	10.801	256.885
CL2	70.90600	-9.181	-9.181	0.000	33.949	9.181	223.082
CL2O	86.90540	67.305	80.826	79.000	47.811	11.695	267.951
Co	58.93320	422.082	426.853	428.442	23.024	6.360	179.520
Co+	58.93265	1186.712	1185.285	1193.003	22.271	6.292	178.348
Co-	58.93375	352.108	363.076	358.414	22.439	6.307	178.414
Cr	51.99610	391.283	395.340	397.480	20.786	6.197	174.313
Cr+	51.99555	1050.349	1048.209	1056.547	20.786	6.197	173.032
Cr-	51.99665	320.826	331.080	327.023	20.786	6.197	173.032
CrN	66.00280	496.231	504.623	505.009	30.754	8.778	230.556
CrO	67.99550	176.732	185.129	186.581	32.636	9.849	238.593
CrO2	83.99490	-118.737	-106.000	-108.043	41.971	10.694	265.575
CrO3	99.99430	-335.077	-318.000	-322.037	58.658	13.040	269.408
CrO3-	99.99485	-646.275	-623.000	-632.851	60.322	13.424	277.590
Cs	132.90545	70.303	78.014	76.500	20.786	6.197	175.602
Cs+	132.90490	452.204	453.718	458.402	20.786	6.197	169.838
Cs-	132.90600	18.600	32.508	24.797	20.786	6.197	169.839
CsBO2	175.71525	-701.368	-683.763	-686.902	59.435	14.466	315.586
CsBr	212.80945	-217.235	-197.264	-206.829	37.313	10.406	267.534
CsCL	168.35845	-252.360	-240.058	-242.229	36.957	10.131	256.082
CsF	151.90385	-373.860	-361.736	-364.215	35.878	9.645	243.249
CsH	133.91339	107.104	119.049	115.950	31.564	8.846	215.183
CsI	259.80992	-162.870	-148.561	-152.320	37.451	10.550	275.287
CsLi	139.84645	151.805	164.148	162.146	37.389	10.341	247.950
CsNO2	178.91095	-226.320	-205.594	-210.340	61.727	15.980	327.723
CsNO3	194.91035	-335.050	-309.984	-318.486	69.114	16.564	336.035
CsNa	155.89522	115.205	129.376	125.907	37.824	10.702	263.062
CsO	148.90485	27.752	39.803	37.587	39.188	9.835	248.512
CsOH	149.91279	-267.835	-251.550	-256.000	49.724	11.835	254.840
CsRb	218.37325	100.505	115.705	111.477	38.072	10.972	283.888
Cs2	265.81090	98.375	113.797	109.404	38.255	11.029	284.682
Cs2Br2	425.61890	-587.942	-548.000	-565.829	82.438	22.113	413.799
Cs2CO3	325.81980	-827.627	-798.131	-806.448	92.044	21.179	388.527
Cs2CL2	336.71690	-665.603	-641.000	-644.658	81.623	20.945	384.584
Cs2F2	303.80771	-911.247	-887.000	-891.859	79.717	19.389	358.063
Cs2I2	519.61984	-476.618	-448.000	-454.033	82.678	22.585	431.190
Cs2O	281.81030	-156.945	-137.183	-142.855	54.545	14.090	324.133
Cs2O+	281.80975	269.252	282.817	283.700	55.396	14.448	332.946
Cs2O2	297.80970	-264.496	-240.393	-247.069	73.070	17.426	340.960
Cs2O2H2	299.82558	-676.937	-644.367	-653.000	108.293	23.937	381.267
Cs2SO4	361.87350	-1141.640	-1104.446	-1117.652	110.165	23.988	411.179

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Cu	63.54600	331.203	336.207	337.400	20.786	6.197	166.399
Cu+	63.54545	1082.882	1081.689	1089.080	20.786	6.197	160.636
Cu-	63.54655	206.521	217.723	212.719	20.786	6.197	160.636
CuCL	98.99900	81.619	91.213	91.090	35.262	9.471	237.210
CuF	82.54440	-21.633	-12.217	-12.550	33.380	9.083	226.498
CuF2	101.54281	-278.996	-265.167	-266.940	47.988	12.056	267.090
CuO	79.54540	296.519	305.863	306.270	35.693	9.751	234.621
Cu2	127.09200	475.410	485.418	485.340	36.585	9.930	241.724
Cu3CL3	296.99700	-287.294	-258.510	-258.570	124.572	28.724	429.533
D	2.01410	215.523	219.807	221.720	20.786	6.197	123.352
D+	2.01355	1534.127	1532.214	1540.324	20.786	6.197	117.585
D-	2.01465	136.555	147.037	142.753	20.786	6.197	117.592
DBr	81.91810	-45.705	-29.160	-37.036	29.228	8.668	204.484
DCL	37.46710	-102.208	-93.333	-93.547	29.170	8.661	192.773
DF	21.01251	-284.866	-276.169	-276.228	29.137	8.638	179.705
DOCL	53.46650	-89.864	-76.648	-79.539	38.585	10.325	240.321
DO2	34.01290	-3.578	9.387	6.487	35.845	10.065	232.883
DO2-	34.01345	-114.875	-95.713	-104.796	36.041	10.080	227.860
D2	4.02820	-8.569	-8.569	0.000	29.195	8.569	144.960
D2+	4.02766	1489.917	1492.289	1498.568	29.510	8.651	156.735
D2-	4.02875	226.447	241.213	235.161	30.315	8.714	158.261
D2O	20.02760	-259.170	-246.261	-249.210	34.265	9.960	198.341
D2O2	36.02700	-155.866	-138.616	-144.300	45.242	11.566	242.098
D2S	36.09320	-34.095	-21.114	-24.007	35.795	10.089	215.316
F	18.99840	72.862	77.274	79.380	22.747	6.518	158.752
F+	18.99785	1760.106	1758.321	1766.816	23.497	6.711	161.730
F-	18.99895	-261.289	-250.680	-255.092	20.786	6.197	145.578
FCN	45.01580	24.199	34.000	34.328	41.757	10.129	224.607
FCO	47.00850	-189.806	-180.000	-179.418	38.880	10.388	248.992
FO	34.99780	99.624	108.377	109.012	31.995	9.388	216.396
FO2, FOO	50.99720	14.144	27.237	25.400	44.453	11.256	259.510
FO2, OFO	50.99720	368.062	381.154	378.600	41.126	10.538	251.289
F2	37.99681	-8.825	-8.825	0.000	31.304	8.825	202.792
F2O	53.99621	13.588	26.754	24.500	43.495	10.912	247.508
F2O2	69.99561	5.422	22.927	19.200	62.073	13.778	277.214
FS2F	102.12681	-351.030	-333.381	-336.435	66.042	14.595	294.087
Fe	55.84500	408.621	413.128	415.471	25.675	6.850	180.490
Fe+	55.84445	1177.282	1175.592	1184.218	26.068	6.936	181.858
Fe-	55.84555	386.696	397.401	393.338	25.023	6.642	180.200
Fe (CO) 5	195.89550	-760.995	-729.521	-727.850	170.705	33.145	439.291
FeCL	91.29800	240.663	249.760	251.040	38.223	10.377	257.576
FeCL2	126.75100	-155.278	-141.590	-141.001	57.571	14.277	299.287
FeCL3	162.20400	-1077.318	-1059.040	-1059.104	77.703	18.214	344.211
FeO	71.84440	242.203	251.050	251.040	31.406	8.837	241.926
Fe (OH) 2	89.85968	-344.745	-323.090	-330.536	71.505	14.209	283.092
Fe2CL4	253.50200	-461.220	-433.843	-431.370	125.876	29.849	464.506
Fe2CL6	324.40800	-694.825	-658.268	-654.378	173.665	40.448	536.945
Ga	69.72300	265.449	271.089	272.000	25.347	6.551	169.045
Ga+	69.72245	850.491	849.934	856.688	20.786	6.197	161.793
GaBr	149.62700	-27.900	-10.000	-17.968	36.557	9.932	251.830
GaBr2	229.53100	-163.206	-133.046	-149.181	55.076	14.025	323.444
GaBr3	309.43500	-312.000	-269.580	-292.963	78.467	19.037	359.416
GaCL	105.17600	-79.231	-69.000	-69.621	35.727	9.609	240.254
GaCL2	140.62900	-234.492	-219.671	-220.979	53.855	13.513	302.930
GaCL3	176.08200	-450.000	-430.588	-432.625	74.777	17.375	324.528

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
GaF	88.72140	-241.690	-231.637	-232.608	33.363	9.081	227.816
GaF2	107.71981	-528.828	-514.363	-516.712	47.811	12.116	278.721
GaF3	126.71821	-936.700	-917.822	-921.477	66.213	15.223	292.183
GaH	70.73094	205.650	215.524	214.323	29.439	8.673	199.779
GaI	196.62747	34.762	47.000	44.871	36.870	10.109	259.781
GaI2	323.53194	-43.426	-24.590	-28.955	55.962	14.471	338.523
GaI3	450.43641	-136.000	-110.566	-115.877	80.205	20.123	384.816
GaO	85.72240	137.899	147.879	146.824	32.226	8.925	230.825
GaOH	86.73034	-154.214	-140.000	-143.630	45.169	10.584	235.153
Ga2Br2	299.25400	-157.757	-121.957	-136.964	81.379	20.793	379.766
Ga2Br4	459.06200	-446.412	-386.092	-415.820	127.693	30.592	471.809
Ga2Br6	618.87000	-714.840	-630.000	-673.689	174.122	41.151	568.127
Ga2CL2	210.35200	-240.461	-220.000	-220.973	79.726	19.488	353.537
Ga2CL4	281.25800	-629.642	-600.000	-602.327	122.739	27.315	419.676
Ga2CL6	352.16400	-998.823	-960.000	-962.464	165.885	36.360	492.759
Ga2F2	177.44281	-623.379	-603.274	-606.231	75.221	17.148	320.316
Ga2F4	215.43961	-1347.656	-1318.726	-1325.003	110.133	22.653	369.066
Ga2F6	253.43642	-2047.755	-2010.000	-2017.624	146.582	30.131	426.411
Ga2I2	393.25494	-7.977	16.499	13.521	82.003	21.498	399.064
Ga2I4	647.06388	-191.852	-154.180	-159.268	130.064	32.584	509.437
Ga2I6	900.87282	-360.868	-310.000	-317.295	177.309	43.573	616.298
Ga2O	155.44540	-111.620	-96.000	-99.457	48.462	12.163	284.141
Ge	72.64000	360.401	365.038	367.800	30.733	7.399	167.914
Ge+	72.63945	1128.779	1127.218	1134.984	21.025	6.206	168.098
Ge-	72.64055	238.422	249.255	245.403	21.985	6.981	180.836
GeBr	152.54400	127.574	144.470	137.438	37.250	9.864	257.228
GeBr2	232.44800	-75.156	-46.000	-60.963	55.757	14.193	319.173
GeBr3	312.35200	-137.581	-96.164	-119.031	78.139	18.549	363.176
GeBr4	392.25600	-314.963	-261.287	-291.000	101.687	23.963	396.196
GeCL	108.09300	59.431	68.658	69.030	36.990	9.599	245.907
GeCL2	143.54600	-184.277	-170.459	-171.000	53.785	13.277	295.835
GeCL3	178.99900	-284.510	-266.102	-266.951	76.258	17.559	335.213
GeCL4	214.45200	-521.137	-498.138	-500.000	95.919	21.137	348.403
GeF	91.63840	-79.737	-70.688	-70.593	34.784	9.144	234.014
GeF2	110.63681	-585.787	-572.326	-574.000	47.848	11.787	270.791
GeF3	129.63521	-821.011	-803.137	-806.333	66.181	14.678	297.728
GeF4	148.63361	-1207.443	-1185.156	-1190.150	81.603	17.293	301.936
GeH4	76.67176	(a)	(a)	90.793	45.017	(a)	217.264
GeI	199.54447	200.964	212.198	210.969	37.083	10.005	264.745
GeO	88.63940	-46.476	-37.500	-37.694	30.804	8.782	223.894
GeO2	104.63880	-117.430	-104.114	-106.172	47.061	11.258	241.255
GeS	104.70500	83.384	92.432	92.525	33.710	9.141	235.582
GeS2	136.77000	105.750	119.210	118.818	54.755	13.068	266.900
Ge2	145.28000	460.803	470.076	471.499	41.681	10.696	256.458
H	1.00794	211.801	216.035	217.999	20.786	6.197	114.718
H+	1.00739	1530.049	1528.085	1536.246	20.786	6.197	108.948
H-	1.00849	132.834	143.265	139.031	20.786	6.197	108.961
HALO	43.98888	-8.114	5.000	1.821	40.996	9.935	219.696
HALO2	59.98828	-367.454	-350.000	-355.474	51.256	11.981	254.826
HBO	27.81834	-219.788	-210.000	-210.621	35.307	9.167	202.696
HBO+	27.81779	1166.125	1169.716	1175.220	34.745	9.095	214.568
HBO2	43.81774	-571.128	-557.000	-560.210	44.295	10.918	240.817
HBS	43.88394	40.922	50.782	50.208	36.740	9.286	214.955
HBS+	43.88339	1119.323	1122.986	1129.459	41.255	10.136	226.304
HBr	80.91194	-44.938	-28.444	-36.290	29.141	8.648	198.700

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			$S^{\circ}(T)$ J/K-mol
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	
HCN	27.02534	123.847	133.470	133.082	35.857	9.235	201.824
HCO	29.01804	32.408	42.036	42.398	34.591	9.989	224.336
HCO+	29.01749	823.988	827.418	833.034	34.172	9.046	201.764
HCCN	39.03604	598.565	609.241	610.431	54.238	11.866	240.596
HCCO	41.02874	164.903	175.584	176.568	49.975	11.665	246.408
HCL	36.46094	-100.950	-92.125	-92.310	29.136	8.640	186.903
HD	3.02204	-8.186	0.333	0.323	29.200	8.509	143.801
HD+	3.02149	1488.179	1490.500	1496.793	29.334	8.614	155.552
HDO	19.02144	-255.206	-242.348	-245.280	33.798	9.926	199.517
HDO2	35.02084	-151.577	-134.378	-140.242	43.779	11.335	243.581
HF	20.00634	-281.899	-273.252	-273.300	29.137	8.599	173.777
HI	127.91241	17.703	28.535	26.359	29.157	8.656	206.592
HNC	27.02534	184.377	194.000	194.378	40.271	10.001	205.511
HNCO	43.02474	-129.023	-115.060	-118.057	45.078	10.966	238.265
HNO	31.01404	92.091	105.000	102.033	33.880	9.942	220.920
HNO2	47.01344	-90.049	-72.800	-78.452	46.320	11.597	254.071
HNO3	63.01284	-145.789	-124.200	-133.913	54.109	11.876	266.878
HOCL	52.46034	-85.965	-72.800	-75.740	37.293	10.225	236.567
HOF	36.00574	-106.987	-94.000	-96.898	35.940	10.088	226.757
HO2	33.00674	2.018	14.932	12.020	34.893	10.002	229.106
HO2-	33.00729	-108.1684	-89.057	-97.923	37.720	10.245	226.610
HPO	47.98110	-66.934	-53.000	-56.869	35.829	10.065	235.683
HSO3F	100.06954	-768.134	-742.055	-753.120	75.245	15.014	297.272
H2	2.01588	-8.468	-8.468	0.000	28.836	8.468	130.681
H2+	2.01533	1486.089	1488.360	1494.672	29.289	8.583	142.370
H2-	2.01643	226.548	241.213	235.168	29.556	8.621	143.747
HBOH	28.82628	-59.665	-45.643	-48.724	43.082	10.941	234.021
HCHO, formaldehy	30.02598	-118.600	-104.738	-108.580	35.388	10.020	218.764
HCOOH	46.02538	-389.498	-371.296	-378.570	45.680	10.928	248.990
H2F2	40.01269	-583.793	-566.500	-569.924	58.132	13.869	260.905
H2O	18.01528	-251.730	-238.922	-241.826	33.588	9.904	188.829
H2O+	18.01473	971.667	978.278	981.602	33.683	9.934	195.378
H2O2	34.01468	-147.039	-129.891	-135.880	42.388	11.159	234.527
H2S	34.08088	-30.558	-17.678	-20.600	34.255	9.958	205.816
H2SO4	98.07848	-749.240	-719.000	-732.732	84.401	16.509	299.289
H2BOH	29.83422	-300.256	-282.000	-289.634	42.642	10.622	230.910
HB (OH) 2	45.83362	-656.596	-634.000	-644.439	57.145	12.158	257.009
H3BO3	61.83302	-1017.920	-990.984	-1004.360	70.040	13.560	268.230
H3B3O3	83.45502	-1219.364	-1190.000	-1203.761	80.615	15.603	286.152
H3B3O6	131.45322	-2287.384	-2245.000	-2263.688	133.912	23.697	359.908
H3F3	60.01903	-898.940	-873.000	-883.677	73.884	15.263	280.947
H3O+	19.02267	587.954	598.798	598.000	35.485	10.046	193.139
(HCOOH) 2	92.05076	-840.575	-804.171	-820.943	96.142	19.632	332.785
H4F4	80.02537	-1208.586	-1174.000	-1186.932	104.022	21.654	350.016
H5F5	100.03172	-1518.233	-1475.000	-1490.188	134.161	28.045	417.286
H6F6	120.03806	-1839.880	-1788.000	-1805.545	163.735	34.334	486.619
H7F7	140.04440	-2140.526	-2080.000	-2099.699	194.438	40.827	548.654
He	4.00260	-6.197	-6.197	0.000	20.786	6.197	126.154
He+	4.00205	2372.324	2372.324	2378.521	20.786	6.197	131.915
Hg	200.59000	55.183	64.526	61.380	20.786	6.197	174.972
Hg+	200.58945	1068.446	1071.591	1074.643	20.786	6.197	180.735
HgBr2	360.39800	-106.970	-73.107	-91.312	60.277	15.658	320.227
I	126.90447	100.563	107.161	106.760	20.786	6.197	180.789
I+	126.90392	1115.154	1115.554	1121.351	20.786	6.197	182.644
I-	126.90502	-200.793	-187.998	-194.596	20.786	6.197	169.262

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
IF5	221.89649	-861.044	-832.383	-841.000	102.750	20.044	334.712
IF7	259.89329	-985.623	-948.137	-961.500	135.652	24.123	353.126
I2	253.80894	52.304	65.500	62.420	36.887	10.116	260.687
In	114.81800	234.501	241.111	240.700	20.830	6.199	173.782
In+	114.81745	0.799	1.212	6.996	20.786	6.197	168.014
InBr	194.72200	-64.200	-45.330	-54.116	36.824	10.084	259.617
InBr2	274.62600	-164.153	-133.023	-149.729	55.831	14.424	333.556
InBr3	354.53000	-276.500	-233.110	-256.587	79.889	19.913	373.477
InCL	150.27100	-81.900	-70.699	-72.148	36.138	9.752	248.274
InCL2	185.72400	-215.440	-199.649	-201.483	54.844	13.956	314.208
InCL3	221.17700	-388.000	-367.618	-369.693	76.722	18.307	339.170
InF	133.81640	-202.637	-191.614	-193.420	34.149	9.217	236.248
InF2	152.81481	-469.776	-454.340	-457.187	49.435	12.589	290.910
InF3	171.81321	-879.400	-859.552	-863.080	69.566	16.320	308.291
InH	115.82594	206.333	217.177	215.017	29.583	8.684	207.665
InI	241.72247	16.146	29.354	26.417	37.101	10.271	267.446
InI2	368.62694	-54.373	-34.567	-39.461	56.620	14.913	349.839
InI3	495.53141	-126.288	-99.884	-105.436	81.093	20.852	398.640
InO	130.81740	136.951	147.901	145.993	33.548	9.042	238.914
InOH	131.82534	-135.184	-120.000	-124.447	46.021	10.737	243.709
In2Br2	389.44400	-217.740	-180.000	-196.305	81.936	21.435	398.293
In2Br4	549.25200	-468.307	-406.047	-436.509	128.879	31.798	496.377
In2Br6	709.06000	-671.780	-585.000	-628.683	176.457	43.097	603.457
In2CL2	300.54200	-252.401	-230.000	-232.177	80.698	20.224	372.424
In2CL4	371.44800	-608.582	-577.000	-579.126	125.237	29.457	455.968
In2CL6	442.35400	-920.763	-880.000	-882.340	169.253	38.423	527.664
In2F2	267.63281	-550.274	-528.229	-532.234	77.254	18.040	339.263
In2F4	305.62961	-1309.551	-1278.681	-1284.788	114.222	24.763	400.833
In2F6	343.62642	-1993.567	-1953.872	-1960.000	155.898	33.567	468.351
In2I2	483.44494	-49.872	-23.456	-27.814	82.382	22.058	416.357
In2I4	737.25388	-232.612	-193.000	-199.143	130.687	33.469	529.944
In2I6	991.06282	-364.808	-312.000	-319.720	178.886	45.088	644.765
In2O	245.63540	-47.560	-30.000	-34.764	50.591	12.797	301.927
K	39.09830	82.803	89.891	89.000	20.786	6.197	160.342
K+	39.09775	507.810	508.701	514.008	20.786	6.197	154.578
K-	39.09885	28.221	41.506	34.418	20.786	6.197	154.579
KAlF4	142.07345	-1929.278	-1900.000	-1907.857	104.398	21.421	351.969
KBO2	81.90810	-682.114	-665.132	-668.023	58.945	14.091	296.738
KBr	119.00230	-189.360	-170.012	-179.251	36.928	10.109	250.537
KCN	65.11570	67.040	79.516	79.496	50.858	12.456	253.150
KCL	74.55130	-224.460	-212.781	-214.575	36.505	9.885	239.094
KF	58.09670	-337.900	-326.399	-328.445	35.233	9.455	226.630
KH	40.10624	116.604	127.926	125.399	31.049	8.795	198.030
KI	166.00277	-138.700	-125.014	-128.456	37.129	10.244	258.291
KLi	46.03930	160.505	172.225	170.702	37.170	10.197	230.171
KNO2	85.10380	-207.840	-187.737	-192.497	61.132	15.343	302.355
KNO3	101.10320	-331.750	-307.307	-315.833	68.530	15.917	311.473
KNa	62.08807	121.830	135.378	132.404	37.783	10.574	245.845
KO	55.09770	55.252	66.680	64.733	35.352	9.481	241.198
KOH	56.10564	-243.675	-228.013	-232.000	49.185	11.675	238.287
K2	78.19660	115.805	129.981	126.546	37.982	10.741	249.760
K2+	78.19605	513.800	521.778	524.661	38.133	10.861	259.959
K2Br2	238.00460	-559.696	-521.000	-538.744	81.657	20.952	376.376
K2CO3	138.20550	-831.165	-802.915	-811.649	89.939	19.516	345.508
K2C2N2	130.23140	-33.154	-8.201	-8.368	110.264	24.786	373.135

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
K2CL2	149.10260	-635.357	-612.000	-615.394	80.699	19.963	350.390
K2F2	116.19341	-878.001	-855.000	-859.875	77.835	18.126	321.150
K2I2	332.00554	-440.372	-413.000	-418.915	82.040	21.457	393.955
K2O	94.19600	-87.945	-69.429	-74.087	54.180	13.858	286.548
K2O+	94.19545	354.252	366.571	368.390	54.874	14.138	297.123
K2O2	110.19540	-207.856	-185.000	-191.566	70.589	16.290	306.461
K2O2H2	112.21128	-663.385	-632.061	-641.000	105.593	22.385	342.859
K2SO4	174.25920	-1118.135	-1082.187	-1095.851	108.055	22.284	364.963
Kr	83.80000	-6.197	-6.197	0.000	20.786	6.197	164.086
Kr+	83.79945	1350.756	1350.756	1356.954	20.786	6.197	175.613
Li	6.94100	153.103	157.735	159.300	20.786	6.197	138.783
Li+	6.94045	679.522	677.957	685.719	20.786	6.197	133.018
Li-	6.94155	87.277	98.107	93.475	20.786	6.197	133.020
LiALF4	109.91615	-1876.822	-1850.000	-1857.288	99.340	19.534	326.521
LiBO2	49.75080	-665.780	-651.254	-652.352	57.163	13.428	272.380
LiBr	86.84500	-160.336	-143.444	-151.163	33.932	9.173	224.337
LiCL	42.39400	-202.840	-193.617	-193.780	33.254	9.060	212.860
LiF	25.93940	-349.773	-340.728	-340.945	31.292	8.828	200.300
LiH	7.94894	130.578	139.444	139.264	29.731	8.686	170.907
LiI	133.84547	-94.560	-83.330	-85.270	34.551	9.290	232.220
LiN	20.94770	325.721	334.688	334.720	32.839	8.999	208.248
LiNO2	52.94650	-215.400	-197.753	-202.031	56.959	13.369	265.014
LiNO3	68.94590	-325.500	-303.513	-311.585	64.061	13.915	278.287
LiO	22.94040	63.552	72.524	72.914	32.317	9.362	211.123
LiOF	41.93880	-102.875	-89.491	-92.048	43.032	10.827	246.026
LiOH	23.94834	-240.337	-227.131	-229.000	46.026	11.337	214.377
LiON	36.94710	168.611	181.918	179.912	44.424	11.301	245.335
Li2	13.88200	206.225	215.489	215.900	36.103	9.675	197.000
Li2+	13.88145	711.622	714.689	721.611	36.978	9.989	207.572
Li2Br2	173.69000	-512.784	-479.000	-495.834	75.105	16.950	317.489
Li2CL2	84.78800	-613.445	-595.000	-597.539	72.625	15.906	292.645
Li2F2	51.87881	-949.089	-931.000	-935.323	64.770	13.766	261.916
Li2I2	267.69094	-380.460	-358.000	-362.801	76.762	17.659	334.607
Li2O	29.88140	-180.131	-166.527	-167.339	50.286	12.792	232.985
Li2O+	29.88085	426.066	433.473	439.095	51.385	13.029	242.552
Li2O2	45.88080	-292.946	-275.002	-279.398	59.412	13.548	258.643
Li2O2H2	47.89668	-752.579	-726.167	-737.000	79.887	15.579	270.726
Li2SO4	109.94460	-1061.469	-1030.432	-1041.816	101.805	19.653	322.826
Li3+	20.82245	743.301	751.000	756.591	54.285	13.289	245.270
Li3Br3	260.53500	-850.676	-800.000	-824.639	118.950	26.037	401.354
Li3CL3	127.18200	-1000.668	-973.000	-976.107	115.506	24.561	367.816
Li3F3	77.81821	-1545.134	-1518.000	-1524.597	102.920	20.537	316.818
Li3I3	401.53641	-639.690	-606.000	-612.457	121.601	27.233	425.290
Mg	24.30500	140.903	145.882	147.100	20.786	6.197	148.649
Mg+	24.30445	884.850	883.631	891.047	20.786	6.197	154.412
MgBr	104.20900	-3.425	13.814	6.163	35.664	9.588	244.976
MgBr2	184.11300	-321.500	-292.001	-306.743	58.550	14.757	296.432
MgCL	59.75800	-64.068	-54.498	-54.705	34.837	9.363	233.423
MgCL+	59.75745	636.824	640.196	646.339	35.447	9.516	228.559
MgCL2	95.21100	-413.070	-398.910	-399.170	56.548	13.901	272.242
MgF	43.30340	-241.236	-231.844	-232.267	32.580	8.969	221.097
MgF+	43.30285	507.898	511.093	516.868	32.606	8.969	215.334
MgF2	62.30181	-748.120	-734.316	-735.498	52.293	12.622	247.556
MgF2+	62.30126	570.277	577.884	582.692	52.450	12.415	258.148
MgH	25.31294	221.104	230.317	229.786	29.587	8.682	193.197

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
MgI	151.20947	51.465	63.042	61.206	36.078	9.741	252.815
MgI2	278.11394	-187.000	-168.825	-171.706	59.364	15.294	313.820
MgN	38.31170	279.707	289.021	288.696	32.733	8.989	224.838
MgO	40.30440	23.352	32.671	32.261	32.111	8.909	213.318
MgOH	41.31234	-143.553	-130.000	-132.429	46.497	11.124	232.622
MgOH+	41.31179	605.581	612.937	615.769	43.216	10.188	220.827
Mg (OH) 2	58.31968	-569.127	-547.000	-551.996	80.668	17.132	271.597
MgS	56.37000	111.415	120.806	120.649	34.237	9.234	225.447
Mg2	48.61000	276.971	286.930	286.513	24.199	9.542	240.843
Mg2F4	124.60361	-1739.512	-1711.904	-1718.369	107.502	21.143	337.018
Mn	54.93805	276.203	281.197	282.400	20.786	6.197	173.718
Mn+	54.93750	999.674	998.470	1005.871	20.786	6.197	175.000
Mo	95.94000	652.303	656.888	658.500	20.786	6.197	181.953
Mo+	95.93945	1342.815	1341.203	1349.013	20.786	6.197	180.671
Mo-	95.94055	574.127	584.910	580.325	20.786	6.197	180.671
MoO	111.93940	347.752	356.677	358.005	35.432	10.253	244.759
MoO2	127.93880	-26.265	-13.000	-15.558	42.011	10.707	273.915
MoO3	143.93820	-377.605	-360.000	-364.412	59.516	13.193	276.516
MoO3-	143.93875	-668.803	-645.000	-655.243	60.762	13.560	284.670
Mo2O6	287.87640	-1175.210	-1140.000	-1149.447	130.228	25.763	387.433
Mo3O9	431.81460	-1942.815	-1890.000	-1902.031	205.375	40.784	508.711
Mo4O12	575.75280	-2680.421	-2610.000	-2625.527	280.018	54.894	609.496
Mo5O15	719.69100	-3398.026	-3310.000	-3329.108	353.826	68.917	709.311
N	14.00670	466.483	470.818	472.680	20.786	6.197	153.302
N+	14.00615	1875.011	1873.149	1882.128	21.285	7.117	159.799
N-	14.00725	467.039	477.572	473.538	21.009	6.498	159.930
NCO	42.01680	121.649	131.378	131.847	39.989	10.198	232.229
ND	16.02080	347.091	355.710	355.739	29.159	8.648	187.234
ND2	18.03490	174.874	187.778	184.837	34.415	9.962	204.335
ND3	20.04901	-64.986	-47.797	-54.752	38.225	10.234	203.931
NF	33.00510	224.252	233.000	232.990	30.228	8.738	213.020
NF2	52.00351	23.840	37.000	34.421	41.058	10.582	249.638
NF3	71.00191	-143.555	-125.982	-131.700	53.497	11.855	260.812
NH	15.01464	348.431	357.000	357.032	29.193	8.601	181.227
NH+	15.01409	1656.293	1658.664	1665.788	32.775	9.495	187.651
NHF	34.01304	101.970	114.952	112.000	35.234	10.030	230.806
NHF2	53.01145	-113.807	-96.413	-103.000	43.384	10.807	252.814
NH2	16.02258	179.197	192.000	189.135	33.857	9.938	194.996
NH2F	35.02098	-85.105	-67.889	-75.000	36.474	10.105	229.534
NH3	17.03052	-55.983	-38.946	-45.940	35.630	10.043	192.770
NH2OH	33.02992	-61.236	-39.859	-50.000	46.472	11.236	236.181
NH4+	18.03791	634.926	650.000	644.905	34.764	9.979	186.095
NO	30.00610	82.092	90.767	91.271	29.862	9.179	210.748
NO+	30.00555	982.140	984.617	990.810	29.123	8.670	198.234
NOCL	65.45910	41.334	54.600	52.699	44.623	11.364	261.590
NOF	49.00450	-75.720	-62.633	-65.000	41.530	10.720	248.224
NOF3	87.00131	-200.698	-178.785	-187.000	68.067	13.698	277.731
NO2	46.00550	23.985	37.000	34.193	37.177	10.208	240.171
NO2-	46.00605	-210.213	-191.000	-200.036	37.215	10.177	236.219
NO2CL	81.45850	0.295	17.901	12.500	53.245	12.205	272.128
NO2F	65.00390	-120.347	-102.919	-109.000	48.999	11.347	259.287
NO3	62.00490	60.169	77.524	71.128	46.935	10.959	252.623
NO3-	62.00545	-321.553	-298.000	-310.780	44.724	10.773	245.638
NO3F	81.00330	0.556	22.324	15.000	66.959	14.444	293.171
N2	28.01340	-8.670	-8.670	0.000	29.124	8.670	191.610



# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
N2+	28.01285	1500.837	1503.310	1509.508	29.137	8.671	197.663
N2-	28.01395	139.509	154.377	148.183	29.194	8.674	204.539
NCN	40.02410	490.276	500.000	500.457	41.946	10.180	225.814
N2D2, cis	32.04160	192.549	209.788	202.857	39.025	10.308	224.095
N2F2	66.01021	49.505	67.000	62.374	56.569	12.869	268.216
N2F4	104.00701	-39.812	-13.491	-22.000	88.384	17.812	317.531
N2H2	30.02928	201.862	219.000	211.859	35.045	9.997	218.333
NH2NO2	62.02808	-38.164	-12.346	-26.000	56.372	12.164	268.548
N2H4	32.04516	83.731	109.337	95.180	48.430	11.449	238.466
N2O	44.01280	72.019	85.029	81.600	38.628	9.581	220.010
N2O+	44.01225	1322.333	1329.146	1332.957	42.263	10.623	233.859
N2O3	76.01160	69.510	91.200	86.631	72.733	17.121	314.736
N2O4	92.01100	-5.630	20.400	11.111	79.168	16.741	304.451
N2O5	108.01040	-7.497	22.873	13.300	95.332	20.797	355.717
N3	42.02010	426.429	439.434	436.000	36.175	9.571	223.071
N3H	43.02804	283.053	300.292	294.000	44.219	10.947	239.330
Na	22.98977	101.303	107.763	107.500	20.786	6.197	153.719
Na+	22.98922	603.346	603.608	609.543	20.786	6.197	147.955
Na-	22.99032	42.256	54.913	48.453	20.786	6.197	147.956
NaAlF4	125.96492	-1878.650	-1850.000	-1857.842	103.092	20.809	341.700
NaBO2	65.79957	-647.132	-630.778	-633.449	58.139	13.683	286.323
NaBr	102.89377	-155.750	-137.030	-145.929	36.338	9.821	241.224
NaCN	49.00717	82.140	93.989	94.266	50.179	12.126	243.370
NaCL	58.44277	-191.160	-180.109	-181.545	35.798	9.615	229.797
NaF	41.98817	-304.382	-293.509	-295.157	34.221	9.225	217.613
NaH	23.99771	132.104	142.798	140.835	30.294	8.731	188.391
NaI	149.89424	-100.590	-87.532	-90.638	36.643	9.952	248.981
NaLi	29.93077	168.605	179.697	178.598	36.910	9.993	219.434
NaNO2	68.99527	-181.100	-161.625	-166.293	60.250	14.807	289.624
NaNO3	84.99467	-300.930	-277.115	-285.529	67.667	15.401	300.084
NaO	38.98917	96.752	107.552	106.505	35.084	9.753	228.583
NaOH	39.99711	-202.398	-187.364	-191.000	47.967	11.398	228.978
NaOH+	39.99656	672.168	681.004	683.862	49.257	11.695	242.630
Na2	45.97954	131.936	144.856	142.339	37.574	10.403	230.246
Na2Br2	205.78754	-500.440	-463.000	-480.848	80.319	19.592	351.048
Na2CL2	116.88554	-583.101	-561.000	-564.402	79.035	18.699	327.529
Na2F2	83.97635	-850.745	-829.000	-834.063	74.929	16.682	297.907
Na2I2	299.78848	-377.116	-351.000	-356.870	81.056	20.246	368.732
Na2O	61.97894	-30.970	-13.710	-16.560	56.773	14.410	271.324
Na2O+	61.97839	506.227	517.290	520.834	57.404	14.607	280.689
Na2O2	77.97834	-139.496	-117.895	-123.930	68.503	15.565	289.595
Na2O2H2	79.99422	-643.346	-613.278	-624.000	97.360	19.346	309.772
Na2SO4	142.04214	-1061.104	-1026.412	-1040.132	105.223	20.972	345.365
Na3CL3	175.32831	-942.152	-909.000	-912.675	126.381	29.477	426.719
Na3F3	125.96452	-1373.618	-1341.000	-1348.015	119.035	25.602	372.029
Nb	92.90638	714.759	720.000	723.113	30.159	8.354	186.262
Nb+	92.90583	1385.016	1384.059	1393.605	30.291	8.589	182.978
Nb-	92.90693	622.400	633.839	631.054	28.948	8.654	186.097
NbCL5	270.17138	-729.673	-701.479	-703.330	119.042	26.343	404.118
NbO	108.90578	202.209	211.790	210.989	30.784	8.780	238.972
NbOCL3	215.26478	-772.931	-749.578	-752.300	92.002	20.631	358.302
NbO2	124.90518	-211.921	-198.000	-201.267	41.514	10.654	269.934
Ne	20.17970	-6.197	-6.197	0.000	20.786	6.197	146.330
Ne+	20.17915	2080.662	2080.662	2086.966	22.120	6.304	158.310
Ni	58.69340	423.292	428.078	430.117	23.361	6.825	182.193

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Ni+	58.69285	1166.389	1164.977	1172.595	20.990	6.206	174.574
Ni-	58.69395	305.557	316.541	311.764	21.018	6.207	174.580
NiCL	94.14640	172.539	181.916	182.004	35.444	9.465	251.887
NiCL2	129.59940	-88.138	-74.170	-73.931	58.078	14.207	294.237
NiO	74.69280	288.197	297.323	297.064	31.701	8.867	231.090
NiS	90.75840	348.200	357.398	357.419	34.452	9.219	252.287
O	15.99940	242.450	246.790	249.175	21.912	6.725	161.060
O+	15.99885	1562.590	1560.732	1568.787	20.786	6.197	154.961
O-	15.99995	95.275	105.813	101.846	21.685	6.571	157.797
OD	18.01350	26.173	34.798	35.172	29.939	8.999	189.668
OD-	18.01405	-156.200	-141.378	-147.558	29.143	8.642	178.411
OH	17.00734	28.465	37.039	37.278	29.886	8.813	183.740
OH+	17.00679	1290.610	1292.987	1299.213	29.196	8.603	182.746
OH-	17.00789	-153.862	-139.091	-145.256	29.141	8.606	172.542
O2	31.99880	-8.680	-8.680	0.000	29.378	8.680	205.149
O2+	31.99825	1162.517	1165.000	1171.828	30.670	9.311	205.392
O2-	31.99935	-57.378	-42.500	-48.028	31.422	9.350	209.336
O3	47.99820	131.434	144.454	141.800	39.376	10.366	239.010
P	30.97376	310.303	315.663	316.500	20.786	6.197	163.200
P+	30.97321	1328.312	1327.474	1336.453	25.859	8.142	166.971
P-	30.97431	232.079	243.636	238.827	22.169	6.748	169.126
PCL	66.42676	125.324	135.275	134.615	33.991	9.291	236.883
PCL2	101.87976	-66.541	-52.000	-54.292	50.935	12.249	285.127
PCL2-	101.88031	-368.738	-348.000	-356.285	50.861	12.453	281.466
PCL3	137.33276	-305.432	-286.301	-289.500	71.592	15.932	311.708
PCL5	208.23876	-399.305	-370.993	-376.000	113.318	23.305	367.209
PF	49.97216	-56.836	-47.063	-47.945	31.619	8.891	225.006
PF+	49.97162	892.088	895.663	901.518	33.429	9.430	224.038
PF-	49.97271	-173.562	-157.592	-164.046	34.786	9.516	225.221
PFCL	85.42516	-294.815	-280.451	-283.184	47.535	11.630	279.494
PFCL-	85.42571	-541.012	-520.451	-529.269	47.800	11.743	274.544
PFCL2	120.87816	-526.793	-507.839	-511.925	67.435	14.868	307.925
PFCL4	191.78416	-656.750	-628.616	-635.016	107.850	21.734	358.036
PF2	68.97057	-524.185	-510.000	-513.104	44.304	11.081	262.183
PF2-	68.97112	-720.383	-700.000	-709.338	44.380	11.045	256.272
PF2CL	104.42357	-748.953	-730.177	-735.077	63.101	13.876	295.068
PF2CL3	175.32957	-898.910	-870.953	-878.745	102.183	20.165	338.132
PF3	87.96897	-970.336	-951.739	-957.400	58.685	12.936	273.060
PF3CL2	158.87497	-1141.070	-1113.291	-1122.023	97.348	19.047	335.435
PF4CL	142.42037	-1383.230	-1355.629	-1364.909	93.005	18.321	326.834
PF5	125.96578	-1609.838	-1582.415	-1593.300	84.703	16.538	301.026
PH	31.98170	222.104	231.698	230.752	29.175	8.648	196.381
PH2	32.98964	109.572	123.400	119.553	34.450	9.982	212.610
PH2-	32.99019	-19.226	0.800	-9.265	34.124	9.960	205.247
PH3	33.99758	-4.698	13.365	5.439	37.102	10.137	210.245
PN	44.98046	162.785	172.480	171.487	29.691	8.702	211.135
PO	46.97316	-37.248	-27.548	-27.858	31.761	9.390	222.744
PO-	46.97371	-148.845	-132.948	-140.067	30.759	8.778	222.403
POCL3	153.33216	-586.116	-562.644	-568.400	84.355	17.716	324.466
POFCL2	136.87756	-810.343	-787.050	-793.889	79.234	16.454	320.344
POF2CL	120.42297	-1037.503	-1014.388	-1022.607	73.066	14.896	305.054
POF3	103.96837	-1266.166	-1243.229	-1252.000	68.874	14.166	285.422
PO2	62.97256	-292.040	-278.000	-281.527	39.524	10.513	253.687
PO2-	62.97311	-608.237	-588.000	-597.624	40.517	10.614	249.406
PS	63.03876	140.815	150.587	150.431	35.242	9.616	234.068

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
P2	61.94752	135.096	145.816	144.000	32.032	8.904	218.124
P2O3	109.94572	-700.740	-677.000	-684.645	73.927	16.095	312.698
P2O4	125.94512	-951.080	-923.000	-933.755	85.131	17.326	312.913
P2O5	141.94452	-1146.420	-1114.000	-1124.370	105.936	22.050	366.580
P3	92.92128	197.994	214.074	210.000	51.873	12.006	263.529
P3O6	188.91768	-1599.120	-1557.000	-1575.681	135.741	23.439	376.077
P4	123.89504	44.791	66.231	58.900	67.081	14.109	279.883
P4O6	219.89144	-1630.798	-1583.317	-1606.000	148.611	24.798	356.395
P4O7	235.89084	-2010.820	-1959.000	-1984.448	159.256	26.372	379.867
P4O8	251.89024	-2330.160	-2274.000	-2302.214	169.902	27.946	394.949
P4O9	267.88964	-2643.500	-2583.000	-2613.979	180.548	29.521	402.497
P4O10	283.88904	-2937.320	-2872.479	-2906.223	191.196	31.097	402.094
Pb	207.20000	189.003	195.873	195.200	20.786	6.197	175.377
Pb+	207.19945	910.799	911.472	916.997	20.786	6.197	181.140
Pb-	207.20055	147.685	160.752	153.882	20.786	6.197	186.903
PbBr	287.10400	54.675	73.805	64.821	36.916	10.146	272.744
PbBr2	367.00800	-118.930	-87.540	-103.908	56.966	15.022	339.673
PbBr3	446.91200	-123.980	-80.330	-104.011	80.540	19.969	385.255
PbBr4	526.81600	-208.307	-152.397	-182.436	104.468	25.871	427.724
PbCL	242.65300	-0.968	10.493	8.819	36.215	9.787	261.306
PbCL2	278.10600	-189.550	-173.499	-175.547	55.299	14.003	315.621
PbCL3	313.55900	-195.909	-175.268	-177.654	77.918	18.256	351.604
PbCL4	349.01200	-350.880	-325.648	-327.430	100.537	23.449	381.682
PbF	226.19840	-108.136	-96.853	-98.868	34.401	9.268	249.962
PbF2	245.19681	-456.000	-440.305	-443.427	50.981	12.573	291.532
PbF3	264.19521	-505.108	-485.000	-489.573	70.582	15.535	316.287
PbF4	283.19361	-819.551	-795.031	-799.925	90.232	19.626	331.825
PbI	334.10447	98.565	112.033	108.904	37.152	10.339	280.413
PbI2	461.00894	-25.500	-5.434	-10.253	57.182	15.247	352.613
PbI3	587.91341	0.690	27.354	21.755	81.624	21.065	411.532
PbI4	714.81788	-68.747	-35.485	-41.226	106.254	27.521	463.806
PbO	223.19940	59.175	70.385	68.137	32.513	8.962	240.045
PbO2	239.19880	123.902	139.452	136.153	51.721	12.251	261.093
PbS	239.26500	118.515	129.797	127.945	35.085	9.430	251.414
PbS2	271.33000	230.028	245.722	244.049	57.511	14.021	286.141
Rb	85.46780	74.703	82.192	80.900	20.786	6.197	170.095
Rb+	85.46725	483.932	485.223	490.129	20.786	6.197	164.332
Rb-	85.46835	21.621	35.308	27.819	20.786	6.197	164.332
RbBO2	128.27760	-693.310	-675.927	-678.977	59.261	14.333	308.301
RbBr	165.37180	-201.830	-182.081	-191.511	37.217	10.319	261.132
RbCL	120.92080	-233.380	-221.300	-223.323	36.836	10.057	249.692
RbF	104.46620	-343.100	-331.198	-333.512	35.710	9.588	237.119
RbH	86.47574	110.504	122.227	119.324	31.305	8.820	208.726
RbI	212.37227	-148.940	-134.853	-138.481	37.372	10.459	268.872
RbK	124.56610	109.205	123.782	120.013	37.894	10.808	266.235
RbLi	92.40880	153.905	166.026	164.181	37.357	10.276	240.928
RbNO2	131.47330	-203.400	-182.896	-187.630	61.564	15.770	317.580
RbNO3	147.47270	-331.340	-306.496	-314.972	68.981	16.368	326.440
RbNa	108.45757	120.805	134.754	131.470	37.879	10.665	256.435
RbO	101.46720	42.152	53.981	52.489	42.496	10.337	244.913
RbOH	102.47514	-249.761	-233.698	-238.000	49.520	11.761	248.502
Rb2Br2	330.74360	-573.498	-534.000	-551.801	82.195	21.697	398.376
Rb2CL2	241.84160	-639.159	-615.000	-618.374	81.442	20.786	374.474
Rb2F2	208.93241	-873.803	-850.000	-854.913	79.075	18.890	342.830
Rb2I2	424.74454	-455.174	-427.000	-432.956	82.508	22.218	416.286

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Rb2O	186.93500	-123.145	-103.827	-108.929	54.827	14.216	307.147
Rb2O2	202.93440	-232.696	-209.037	-215.848	71.934	16.847	326.309
Rb2O2H2	204.95028	-662.407	-630.281	-639.000	107.351	23.407	367.188
Rb2SO4	266.99820	-1119.914	-1083.164	-1096.592	109.390	23.322	392.360
Rn	222.01760	-6.197	-6.197	0.000	20.786	6.197	176.238
Rn+	222.01705	1037.073	1037.073	1043.270	20.786	6.197	187.764
S	32.06500	270.513	274.925	277.170	23.674	6.657	167.832
S+	32.06445	1276.299	1274.514	1282.496	20.786	6.197	163.631
S-	32.06555	63.904	74.513	70.369	22.783	6.465	164.923
SCL	67.51800	146.646	155.648	156.465	37.542	9.819	237.328
SCL2	102.97100	-30.018	-16.425	-17.573	50.896	12.445	281.632
SCL2+	102.97045	888.930	896.326	901.383	50.861	12.453	287.326
SD	34.07910	129.196	137.893	138.491	32.520	9.294	201.488
SF	51.06340	5.975	14.800	15.446	35.180	9.470	225.281
SF+	51.06285	985.706	988.333	994.570	31.679	8.864	225.410
SF-	51.06395	-240.222	-225.200	-231.347	31.787	8.875	216.350
SF2	70.06181	-304.237	-291.000	-293.189	44.415	11.048	256.582
SF2+	70.06126	694.782	701.821	706.016	44.937	11.234	263.528
SF2-	70.06235	-406.920	-387.485	-394.795	50.165	12.125	267.450
SF3	89.06021	-517.650	-500.000	-504.101	63.148	13.548	285.616
SF3+	89.05966	381.174	392.627	393.583	56.224	12.409	268.976
SF3-	89.06076	-803.847	-780.000	-790.124	64.068	13.723	281.593
SF4	108.05861	-775.383	-753.321	-760.000	76.673	15.383	296.713
SF4+	108.05806	399.606	415.471	416.112	80.396	16.506	311.676
SF4-	108.05916	-905.945	-877.685	-887.464	89.189	18.480	312.967
SF5	127.05702	-921.475	-895.000	-902.663	100.085	18.811	322.275
SF5+	127.05647	156.297	176.574	172.644	89.844	16.347	298.156
SF5-	127.05756	-1223.672	-1191.000	-1204.622	101.065	19.050	317.070
SF6	146.05542	-1236.340	-1205.453	-1219.400	97.069	16.940	291.678
SF6-	146.05597	-1359.367	-1322.282	-1341.876	99.986	17.491	302.865
SH	33.07294	133.037	141.683	142.135	32.479	9.098	195.554
SH-	33.07349	-95.220	-80.377	-86.574	29.146	8.646	186.638
SN	46.07170	257.995	266.742	267.388	31.795	9.393	222.095
SO	48.06440	-4.038	4.714	4.760	30.176	8.798	221.941
SO-	48.06495	-115.435	-100.486	-105.968	34.425	9.467	223.678
SOF2	86.06121	-597.577	-580.000	-584.952	57.095	12.625	279.138
SO2	64.06380	-307.358	-294.266	-296.810	39.842	10.548	248.222
SO2-	64.06435	-419.356	-400.066	-408.606	41.795	10.749	256.027
SO2CL2	134.96980	-370.832	-348.559	-354.803	77.096	16.029	311.101
SO2FCL	118.51520	-571.173	-549.078	-556.472	71.593	14.701	302.854
SO2F2	102.06061	-773.490	-751.573	-760.000	65.776	13.490	283.543
SO3	80.06320	-407.588	-390.156	-395.900	50.619	11.688	256.547
S2	64.13000	119.468	128.292	128.600	32.505	9.132	228.166
S2-	64.13055	-46.730	-31.708	-37.132	37.193	9.597	228.429
S2CL2	135.03600	-33.257	-15.252	-16.736	72.776	16.521	327.237
S2F2	102.12681	-415.131	-397.482	-401.413	63.128	13.718	292.832
S2O	80.12940	-67.164	-54.000	-56.035	44.114	11.129	266.967
S3	96.19500	132.764	146.000	144.738	48.964	11.974	276.296
S4	128.26000	121.352	139.000	135.632	65.944	14.280	293.565
S5	160.32500	113.940	136.000	132.993	87.870	19.053	354.086
S6	192.39000	78.528	105.000	101.315	113.155	22.787	357.812
S7	224.45500	85.616	116.500	111.890	133.866	26.274	404.855
S8	256.52000	69.704	105.000	101.277	156.503	31.573	432.545
Sc	44.95591	370.698	375.905	377.700	22.103	7.002	174.788
Sc+	44.95536	1009.983	1008.993	1017.145	21.762	7.162	178.338

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Sc-	44.95646	346.361	357.766	352.559	20.786	6.197	187.196
ScO	60.95531	-63.852	-54.305	-55.065	30.864	8.787	224.550
ScO+	60.95476	552.433	555.783	561.210	30.744	8.777	218.504
ScO2	76.95471	-424.403	-410.516	-413.651	42.467	10.752	262.583
Sc2O	105.91122	-34.754	-20.000	-23.044	46.529	11.710	270.389
Sc2O2	121.91062	-503.705	-484.611	-490.571	56.093	13.134	283.193
Si	28.08550	442.450	445.667	450.000	22.251	7.550	167.982
Si+	28.08495	1235.165	1232.185	1242.508	24.336	7.343	163.429
Si-	28.08605	302.620	312.035	308.818	20.786	6.197	161.979
SiBr	107.98950	165.122	180.600	175.157	38.711	10.035	247.288
SiBr2	187.89350	-64.317	-36.580	-51.000	53.588	13.317	304.721
SiBr3	267.79750	-174.461	-134.464	-157.000	75.234	17.461	351.326
SiBr4	347.70150	-438.114	-385.856	-415.800	97.010	22.314	379.375
SiC	40.09620	725.729	730.000	734.946	31.032	9.217	226.213
SiC2	52.10690	619.676	625.000	631.361	44.227	11.685	252.239
SiCL	63.53850	132.479	140.287	142.363	35.783	9.884	237.840
SiCL2	98.99150	-175.599	-163.200	-163.069	51.274	12.529	281.618
SiCL3	134.44450	-351.989	-335.000	-336.272	70.563	15.717	316.646
SiCL4	169.89750	-681.655	-660.076	-662.200	90.406	19.455	331.452
SiF	47.08390	-34.689	-27.059	-25.233	32.653	9.456	225.790
SiFCL	82.53690	-389.659	-377.439	-377.827	47.494	11.833	275.147
SiF2	66.08231	-604.043	-592.000	-592.838	44.510	11.204	256.588
SiF3	85.08071	-1009.455	-993.000	-996.437	58.730	13.019	279.708
SiF4	104.07911	-1631.146	-1610.278	-1615.780	73.753	15.366	282.810
SiH	29.09344	359.491	366.943	368.636	30.054	9.145	198.054
SiH+	29.09289	1139.017	1140.271	1147.671	29.184	8.654	186.791
SiHBr3	268.80544	-320.745	-276.514	-302.922	80.411	17.823	348.054
SiHCL	64.54644	44.281	56.323	54.946	41.015	10.665	251.334
SiHCL3	135.45244	-512.374	-491.150	-496.222	75.457	16.152	313.722
SiHF	48.09184	-172.887	-161.023	-162.657	37.793	10.230	238.693
SiHF3	86.08865	-1214.353	-1193.663	-1200.808	63.486	13.545	277.272
SiHI3	409.80685	-93.610	-66.365	-74.475	83.886	19.135	375.011
SiH2	30.10138	263.314	275.000	273.333	34.973	10.018	207.483
SiH2Br2	189.90938	-204.644	-168.439	-190.372	65.546	14.272	310.056
SiH2CL2	101.00738	-333.879	-313.012	-320.494	62.175	13.385	286.738
SiH2F2	68.09819	-802.764	-782.254	-790.776	54.269	11.988	262.134
SiH2I2	283.91032	-52.991	-28.110	-38.074	67.981	14.917	326.801
SiH3	31.10932	194.080	210.000	204.357	38.920	10.277	216.498
SiH3Br	111.01332	-90.010	-61.831	-78.241	52.866	11.769	262.470
SiH3CL	66.56232	-153.279	-132.769	-141.838	51.099	11.441	250.765
SiH3F	50.10772	-387.492	-367.159	-376.560	47.197	10.932	238.405
SiH3I	158.01379	-14.170	8.347	-2.092	54.402	12.078	271.026
SiH4	32.11726	24.165	44.319	34.700	42.787	10.535	204.208
SiI	154.98997	253.012	262.828	262.953	39.009	9.941	253.881
SiI2	281.89444	78.673	95.087	92.466	54.625	13.793	320.976
SiN	42.09220	394.932	402.485	403.668	30.281	8.736	216.814
SiO	44.08490	-107.558	-100.000	-98.842	29.901	8.715	211.600
SiO2	60.08430	-332.616	-320.718	-322.073	44.055	10.543	228.724
SiS	60.15050	99.262	106.892	108.194	32.273	8.932	223.675
SiS2	92.21550	-5.181	6.861	7.023	51.814	12.203	254.063
Si2	56.17100	569.899	576.334	580.196	36.265	10.296	238.007
Si2C	68.18170	542.512	550.000	554.094	45.336	11.582	261.900
Si2F6	170.16142	-2409.984	-2377.074	-2383.290	129.879	26.694	391.386
Si2N	70.17770	385.658	396.428	397.480	49.885	11.822	256.491
Si3	84.25650	615.348	625.000	627.867	50.959	12.520	279.184

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			$S^{\circ}(T)$ J/K-mol
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	
Sn	118.71000	294.985	301.308	301.200	21.260	6.215	168.495
Sn+	118.70945	1009.753	1009.878	1015.950	20.786	6.197	174.193
Sn-	118.71055	173.006	185.526	179.496	24.464	6.490	181.197
SnBr	198.61400	65.658	84.241	75.644	36.648	9.986	264.831
SnBr2	278.51800	-133.570	-102.727	-118.975	56.392	14.595	329.048
SnBr3	358.42200	-177.997	-134.894	-158.716	79.523	19.280	373.603
SnBr4	438.32600	-349.260	-293.897	-324.217	103.285	25.043	413.236
SnCL	154.16300	25.015	35.928	34.659	35.836	9.644	253.414
SnCL2	189.61600	-216.330	-200.826	-202.648	54.636	13.682	305.905
SnCL3	225.06900	-309.926	-289.832	-292.372	76.331	17.554	339.854
SnCL4	260.52200	-500.940	-476.255	-478.466	98.401	22.474	366.879
SnF	137.70840	-104.153	-93.418	-95.017	33.701	9.136	241.615
SnF2	156.70681	-523.200	-508.052	-510.957	49.680	12.243	282.130
SnF3	175.70521	-661.430	-641.870	-646.630	67.799	14.800	304.054
SnF4	194.70361	-1043.569	-1019.595	-1024.767	86.601	18.802	319.474
SnI	245.61447	162.548	175.469	172.725	36.986	10.177	272.297
SnI2	372.51894	-22.950	-3.431	-8.067	56.744	14.883	342.708
SnI3	499.42341	-28.327	-2.210	-8.018	80.792	20.309	398.029
SnI4	626.32788	-145.600	-112.885	-118.854	105.468	26.746	448.738
SnO	134.70940	13.037	23.700	21.911	31.761	8.874	232.118
SnO2	150.70880	-0.116	14.888	11.680	49.548	11.796	251.613
SnS	150.77500	101.798	112.533	111.099	34.537	9.301	243.578
SnS2	182.84000	136.011	151.158	149.646	56.436	13.635	277.046
Sn2	237.42000	409.971	422.617	421.344	42.114	11.373	267.314
Sr	87.62000	154.303	160.861	160.500	20.786	6.197	164.642
Sr+	87.61945	709.969	710.330	716.166	20.786	6.197	170.405
SrBr	167.52400	-74.025	-55.207	-63.918	36.865	10.107	263.877
SrBr2	247.42800	-423.060	-391.982	-406.726	61.239	16.335	326.410
SrCL	123.07300	-137.668	-126.519	-127.868	36.260	9.800	252.470
SrCL+	123.07245	398.529	403.481	408.112	35.621	9.583	244.740
SrCL2	158.52600	-499.230	-483.491	-484.814	55.767	14.416	314.932
SrF	106.61840	-312.836	-301.865	-303.553	34.473	9.283	239.903
SrF+	106.61785	200.362	205.135	209.468	33.509	9.107	232.600
SrF2	125.61681	-798.063	-782.680	-784.794	52.785	13.270	290.677
SrH	88.62794	210.504	221.296	219.227	30.133	8.723	212.753
SrI	214.52447	-18.135	-4.979	-7.852	37.103	10.283	271.890
SrI2	341.42894	-294.921	-275.166	-278.219	61.595	16.702	341.645
SrO	103.61940	-23.248	-12.349	-14.208	33.089	9.040	230.057
SrO+	103.61885	619.950	624.651	630.054	35.190	10.104	244.840
SrOH	104.62734	-205.132	-190.000	-194.086	47.064	11.047	248.661
SrOH+	104.62679	299.065	308.000	310.170	47.341	11.105	243.763
Sr(OH) 2	121.63468	-613.706	-590.000	-596.695	78.877	17.012	309.408
SrS	119.68500	94.815	105.785	104.351	35.480	9.536	243.111
Sr2	175.24000	296.205	309.322	307.570	36.516	11.365	278.279
Ta	180.94790	776.319	782.000	782.519	20.858	6.200	185.221
Ta+	180.94735	1543.341	1542.825	1549.679	23.109	6.338	183.387
Ta-	180.94845	739.053	750.932	745.469	24.561	6.416	174.563
TaCL5	358.21290	-791.704	-763.070	-764.835	120.139	26.869	412.979
TaO	196.94730	233.769	243.790	242.535	30.600	8.766	241.118
TaO2	212.94670	-184.361	-170.000	-173.662	41.795	10.699	277.388
Ti	47.86700	465.461	470.285	473.000	24.430	7.539	180.296
Ti+	47.86645	1129.724	1128.351	1137.624	26.186	7.900	183.591
Ti-	47.86755	451.641	462.663	459.204	22.835	7.563	183.714
TiCL	83.32000	141.170	150.585	150.851	27.300	9.681	249.219
TiCL2	118.77300	-250.775	-236.770	-237.230	57.504	13.545	278.340

# Appendix B (continued)

TABLE B1 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
TiCl3	154.22600	-554.695	-536.099	-539.320	72.568	15.375	316.898
TiCl4	189.67900	-784.774	-761.587	-763.160	95.615	21.614	354.894
TiO	63.86640	39.910	49.075	49.504	31.880	9.593	233.267
TiO+	63.86585	676.108	679.075	685.321	30.941	9.213	229.839
TiOCL	99.31940	-256.405	-242.650	-244.262	51.655	12.143	263.663
TiOCL2	134.77240	-562.262	-543.917	-545.552	71.953	16.710	321.005
TiO2	79.86580	-316.782	-303.278	-305.430	44.087	11.352	260.127
U	238.02891	528.501	534.865	535.000	23.694	6.499	199.790
UF	257.02731	-58.638	-47.861	-49.251	37.949	9.387	251.805
UF+	257.02676	547.560	552.139	557.059	40.248	9.499	251.850
UF-	257.02786	-164.835	-147.861	-155.679	33.802	9.156	250.918
UF2	276.02572	-550.189	-535.000	-535.037	56.172	15.152	315.812
UF2+	276.02517	56.008	65.000	70.446	55.395	14.437	313.999
UF2-	276.02627	-691.387	-670.000	-678.233	55.900	13.153	303.914
UF3	295.02412	-1079.602	-1060.000	-1060.959	76.183	18.643	347.433
UF3+	295.02357	-303.404	-290.000	-284.745	81.735	18.659	338.293
UF3-	295.02467	-1205.799	-1180.000	-1186.441	76.960	19.358	349.245
UF4	314.02252	-1628.050	-1604.036	-1606.157	101.356	21.893	363.179
UF4+	314.02197	-661.853	-644.036	-641.539	91.910	20.313	361.099
UF4-	314.02307	-1750.212	-1720.000	-1728.335	95.803	21.877	372.319
UF5	333.02093	-1973.427	-1945.000	-1949.824	110.637	23.603	386.344
UF5+	333.02038	-877.229	-855.000	-853.617	110.650	23.612	380.630
UF5-	333.02147	-2314.624	-2280.000	-2289.431	120.145	25.193	388.479
UF6	352.01933	-2175.265	-2142.426	-2148.642	129.499	26.623	376.690
UF6-	352.01988	-2719.037	-2680.000	-2691.306	132.268	27.731	392.875
UO	254.02831	20.950	31.654	30.489	42.001	9.538	248.870
UO+	254.02776	572.148	576.654	580.972	31.303	8.824	245.711
UOF	273.02671	-556.188	-541.072	-542.183	53.474	14.005	313.309
UOF2	292.02512	-1133.327	-1113.798	-1115.510	79.293	17.816	336.615
UOF3	311.02352	-1530.465	-1506.523	-1510.638	89.110	19.827	353.073
UOF4	330.02192	-1808.354	-1780.000	-1785.612	108.119	22.743	363.175
UO2	270.02771	-491.280	-476.236	-477.820	59.546	13.460	266.428
UO2+	270.02716	39.917	48.764	51.494	48.698	11.577	261.758
UO2-	270.02826	-587.477	-566.236	-573.700	55.379	13.777	278.453
UO2F	289.02611	-1013.739	-994.282	-997.935	67.978	15.804	328.807
UO2F2	308.02452	-1373.300	-1349.431	-1354.232	86.386	19.068	342.636
UO3	286.02711	-814.384	-795.000	-799.239	64.530	15.145	309.647
UO3-	286.02766	-1320.582	-1295.000	-1305.155	66.105	15.427	318.297
V	50.94150	509.360	514.000	517.267	26.012	7.907	182.301
V+	50.94095	1165.848	1164.290	1173.745	23.150	7.898	183.378
V-	50.94205	452.508	463.345	460.386	23.049	7.878	183.438
VCL4	192.75350	-548.842	-525.839	-527.058	96.045	21.783	366.518
VN	64.94820	514.200	523.175	523.000	31.148	8.800	233.387
VO	66.94090	139.810	148.790	148.583	30.698	8.773	230.903
VO2	82.94030	-243.320	-230.000	-232.698	41.223	10.622	261.997
V4O10	363.76000	-2861.961	-2800.000	-2825.164	218.472	36.796	445.617
W	183.84000	845.027	850.000	851.244	21.306	6.217	173.957
W+	183.83945	1621.620	1620.395	1627.841	21.372	6.221	179.739
W-	183.84055	760.194	771.365	766.392	20.786	6.197	188.782
WCL6	396.55800	-524.503	-491.987	-493.712	143.943	30.791	419.172
WO	199.83940	392.477	401.790	401.736	30.698	9.259	244.227
WOCL4	341.65140	-595.764	-568.089	-573.493	106.140	22.271	377.085
WO2	215.83880	18.347	32.000	29.062	41.980	10.715	271.487
WO2CL2	286.74480	-691.036	-668.202	-671.532	87.200	19.504	353.932
WO3	231.83820	-332.993	-315.000	-319.725	59.164	13.268	283.127

# Appendix B (continued)

TABLE B1 (concluded)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
WO3-	231.83875	-664.191	-640.000	-650.476	61.174	13.715	291.664
(WO3) 2	463.67640	-1235.986	-1200.000	-1210.443	128.395	25.543	395.245
(WO3) 3	695.51460	-2053.979	-2000.000	-2013.291	204.304	40.688	518.322
(WO3) 4	927.35280	-2871.973	-2800.000	-2817.434	276.407	54.539	618.888
(WO3) 5	1159.19100	-3619.966	-3530.000	-3551.492	349.313	68.473	717.875
Xe	131.29300	-6.197	-6.197	0.000	20.786	6.197	169.686
Xe+	131.29245	1170.355	1170.355	1176.552	20.786	6.197	181.213
Zn	65.39000	124.203	129.860	130.400	20.786	6.197	160.993
Zn+	65.38945	1036.803	1036.262	1043.000	20.786	6.197	166.756
Zr	91.22400	592.503	598.000	599.319	26.642	6.816	181.346
Zr+	91.22345	1238.774	1238.074	1246.246	28.283	7.472	183.642
Zr-	91.22455	545.203	556.897	552.952	28.693	7.749	185.765
ZrN	105.23070	704.509	714.341	713.372	31.661	8.863	233.491
ZrO	107.22340	74.953	84.790	83.923	34.374	8.970	228.187
ZrO+	107.22285	711.150	714.790	720.614	33.471	9.464	236.915
ZrO2	123.22280	-329.051	-314.874	-317.043	46.062	12.008	273.750
Air	28.96512	-8.775	-0.125	-0.126	29.102	8.649	198.822
CLO3F	102.44960	-37.099	-15.076	-23.800	64.925	13.299	278.989
JP-10 (g)	136.23404	-109.853	-31.574	-86.856	152.560	22.997	359.201
Jet-A (g)	167.31102	(a)	(a)	-249.657	293.491	(a)	628.437

<sup>a</sup> No data available for 0 K.



## Appendix B (continued)

**TABLE B2.—THERMODYNAMIC PROPERTIES FOR CONDENSED SPECIES AT 0 AND 298.15 K**

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Ag (cr)	107.86820	-5.745	-5.745	0.000	25.350	5.745	42.550
Al (cr)	26.98154	-4.540	-4.540	0.000	24.200	4.540	28.300
AlBr3 (cr)	266.69354	-533.420	-492.100	-511.500	100.562	21.920	180.250
ALCL3 (cr)	133.33964	-722.080	-703.768	-705.100	91.133	16.980	109.290
ALF3 (II)	83.97675	-1522.020	-1504.243	-1510.400	75.122	11.620	66.500
ALH3 (a)	30.00536	-16.840	0.402	-11.400	40.210	5.440	30.040
ALI3 (cr)	407.69495	-325.200	-300.866	-302.900	98.893	22.300	190.000
ALN (cr)	40.98828	-322.870	-313.995	-319.000	30.087	3.870	20.170
AL (OH) 3 (a)	78.00356	-1305.960	-1275.698	-1293.500	91.969	12.460	68.440
AL2O3 (a)	101.96128	-1685.716	-1663.616	-1675.700	79.033	10.016	50.920
AL2S3 (a)	150.16108	-667.130	-644.814	-648.500	105.060	18.630	116.860
AL2SiO5 (an)	162.04558	-2609.165	-2575.167	-2592.072	122.755	17.093	93.221
AL4C3 (cr)	143.95825	-223.370	-202.049	-206.900	116.779	16.470	88.950
B (b)	10.81100	-1.214	-1.214	0.000	11.315	1.214	5.834
BN (cr)	24.81774	-253.628	-248.079	-251.000	19.705	2.628	14.810
B2O3 (cr)	69.62020	-1282.801	-1267.353	-1273.500	62.761	9.301	53.970
B2S3 (cr)	117.82000	-260.200	-244.536	-243.000	111.724	17.200	100.000
B3O3H3 (cr)	83.45502	(a)	(a)	-1262.313	98.324	(a)	167.360
B4C (cr)	55.25470	-67.611	-61.702	-62.000	53.090	5.611	27.110
Ba (cr)	137.32700	-6.907	-6.907	0.000	28.110	6.907	62.352
BaBr2 (cr)	297.13500	-771.000	-739.573	-752.000	75.942	19.000	150.000
BaCO3 (a)	197.33590	-1230.510	-1209.530	-1214.000	85.983	16.510	112.100
BaCl2 (a)	208.23240	-871.900	-855.812	-855.200	75.140	16.700	123.700
BaF2 (a)	175.32381	-1220.440	-1204.708	-1206.000	71.129	14.440	96.360
BaH2 (a)	139.34288	-199.100	-183.725	-190.000	46.000	9.100	63.000
BaI2 (cr)	391.13594	-625.230	-605.127	-606.000	77.488	19.230	165.200
BaO (cr)	153.32640	-557.962	-546.715	-548.000	47.020	9.962	72.000
Ba (OH) 2 (b)	171.34168	-956.748	-932.693	-940.600	89.080	16.148	107.280
BaS (cr)	169.39300	-480.820	-469.501	-470.000	49.370	10.820	78.450
BaSO4 (a)	233.39060	-1489.180	-1460.501	-1470.000	102.096	19.180	132.100
Be (a)	9.01218	-1.942	-1.942	0.000	16.443	1.942	9.503
BeAL2O4 (cr)	126.97286	-2313.870	-2285.488	-2300.782	105.380	13.088	66.291
BeBr2 (cr)	168.82018	-372.900	-346.438	-358.000	69.454	14.900	108.000
BeCO3 (cr)	69.02108	-1054.200	-1038.185	-1045.000	64.995	9.200	52.000
BeCL2 (a)	79.91758	-507.620	-496.497	-496.200	62.421	11.420	75.810
BeF2 (a)	47.00899	-1035.468	-1024.701	-1027.000	51.840	8.468	53.350
BeI2 (cr)	262.82112	-206.200	-191.062	-191.000	71.128	15.200	121.000
BeO (a)	25.01158	-612.237	-605.955	-609.400	25.565	2.837	13.770
Be (OH) 2 (b)	43.02686	-913.993	-894.903	-905.700	62.132	8.293	45.480
BeS (cr)	41.07818	-241.500	-235.146	-236.000	33.998	5.500	34.000
BeSO4 (a)	105.07578	-1212.970	-1189.256	-1200.000	85.689	12.970	77.910
Be2C (cr)	30.03506	(a)	(a)	-116.985	43.264	(a)	16.318
Be3N2 (a)	55.05003	-595.124	-580.628	-588.000	64.757	7.124	34.400
Br2 (cr)	159.80800	-24.520	-24.520	0.000	75.680	24.520	152.210
C (gr)	12.01070	-1.054	-1.054	0.000	8.528	1.054	5.734
Ca (a)	40.07800	-5.783	-5.783	0.000	25.750	5.783	42.536
CaBr2 (cr)	199.88600	-700.800	-670.498	-683.800	75.061	17.000	130.000
CaCO3 (cr)	100.08690	-1221.080	-1201.224	-1206.600	83.472	14.480	91.710
CaCL2 (cr)	110.98340	-811.100	-796.136	-795.800	72.846	15.300	108.400
CaF2 (a)	78.07481	-1239.640	-1225.032	-1228.000	67.027	11.640	68.450

# Appendix B (continued)

TABLE B2 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
CaH2 (a)	42.09388	-183.770	-169.519	-177.000	41.000	6.770	41.400
CaI2 (cr)	293.88694	-554.370	-535.392	-536.400	76.986	17.970	145.300
CaO (cr)	56.07740	-641.670	-631.548	-634.920	42.050	6.751	38.100
Ca (OH) 2 (cr)	74.09268	-1000.060	-977.129	-985.900	87.488	14.160	83.400
CaS (cr)	72.14400	-484.010	-473.816	-475.000	47.449	9.010	56.500
CaSO4 (II)	136.14160	-1451.200	-1423.645	-1434.000	99.660	17.201	107.000
Cd (cr)	112.41100	-6.247	-6.247	0.000	26.020	6.247	51.800
Co (a)	58.93320	-4.771	-4.771	0.000	24.802	4.771	30.067
Cr (cr)	51.99610	-4.057	-4.057	0.000	23.434	4.057	23.618
CrN (cr)	66.00284	-124.857	-116.465	-117.152	52.677	7.705	37.711
Cr2N (cr)	117.99894	(a)	(a)	-125.520	66.065	(a)	64.852
Cr2O3 (I')	151.99040	-1155.900	-1134.766	-1140.600	120.080	15.300	81.100
Cs (cr)	132.90545	-7.711	-7.711	0.000	32.210	7.711	85.230
CsBO2 (cr)	175.71525	-976.368	-958.763	-962.000	80.580	14.368	104.350
CsBr (cr)	212.80945	-418.735	-398.764	-405.600	52.930	13.135	112.940
CsCL (a)	168.35815	-454.760	-442.458	-442.310	52.470	12.450	101.170
CsF (cr)	151.90385	-568.860	-556.736	-557.100	51.090	11.760	92.960
CsH (cr)	133.91339	-64.540	-52.595	-54.040	40.600	10.500	73.000
CsI (cr)	259.80992	-361.570	-347.261	-348.100	52.470	13.470	122.200
CsNO2 (I)	178.91099	-403.320	-382.594	-379.900	91.340	23.420	174.000
CsNO3 (a)	194.91039	-525.050	-499.984	-505.000	96.140	20.050	153.830
CsOH (b)	149.91279	-430.303	-414.018	-416.200	69.930	14.103	104.220
CsO2 (a)	164.90425	-304.100	-287.709	-286.100	79.000	18.000	142.000
Cs2CO3 (cr)	325.81980	-1160.627	-1131.131	-1134.900	123.850	25.727	204.470
Cs2O (cr)	281.81030	-364.080	-344.318	-346.400	76.000	17.680	146.900
Cs2O2 (cr)	297.80970	-461.300	-437.198	-440.000	95.000	21.300	180.000
Cs2SO4 (a)	361.87450	-1470.640	-1433.446	-1442.900	134.892	27.740	211.910
Cu (cr)	63.54600	-5.004	-5.004	0.000	24.440	5.004	33.150
CuBr (a)	143.45000	(a)	(a)	-105.604	54.743	(a)	96.102
CuBr2 (cr)	223.35400	(a)	(a)	-138.490	75.740	(a)	128.867
CuCL (a)	98.99870	(a)	(a)	-155.645	52.534	(a)	87.743
CuCL2 (cr)	134.45140	(a)	(a)	-217.986	71.873	(a)	108.073
CuF (cr)	82.54440	(a)	(a)	-209.200	51.882	(a)	64.852
CuF2 (cr)	101.54281	(a)	(a)	-539.820	66.162	(a)	78.032
CuI (a)	190.45047	-79.960	-68.358	-67.781	54.057	12.180	96.596
CuO (cr)	79.54540	-162.745	-153.401	-155.645	42.296	7.100	42.635
Cu (OH) 2 (cr)	97.56068	(a)	(a)	-443.086	87.864	(a)	87.027
CuS (cr)	95.61200	(a)	(a)	-55.647	47.380	(a)	67.166
CuSO4 (cr)	159.60960	-785.471	-758.694	-768.601	98.876	16.870	109.508
Cu2O (cr)	143.09140	-183.305	-168.957	-170.707	62.593	12.598	92.395
Cu2S (a)	159.15800	(a)	(a)	-75.730	76.910	(a)	116.152
Fe (a)	55.84500	-4.507	-4.507	0.000	25.094	4.507	27.321
Fe (CO) 5 (L)	195.89550	-819.024	-787.550	-766.090	233.785	52.934	337.078
FeCL2 (cr)	126.75040	-358.106	-344.418	-341.833	76.664	16.273	117.947
FeCL3 (cr)	162.20310	-418.678	-400.399	-399.237	96.943	19.441	147.821
Fe.9470 (cr)	68.88461	(a)	(a)	-266.270	47.990	(a)	57.488
FeOCL (cr)	107.29710	-423.935	-410.497	-410.994	70.501	12.940	82.551
Fe (OH) 2 (cr)	89.85968	(a)	(a)	-574.045	97.069	(a)	87.864
Fe (OH) 3 (cr)	106.86702	(a)	(a)	-832.616	101.671	(a)	104.600
FeS (a)	87.91100	-109.035	-100.116	-99.621	50.543	9.414	60.312
FeSO4 (cr)	151.90860	-945.617	-919.338	-928.848	100.583	16.769	120.955
FeS2 (cr)	119.97700	-181.185	-167.854	-171.544	62.124	9.641	52.915
Fe2O3 (cr)	159.68820	(a)	(a)	-824.248	103.763	(a)	87.404
Fe2 (SO4) 3 (cr)	399.88080	(a)	(a)	-2582.992	264.722	(a)	307.524
Fe3O4 (cr)	231.53260	-1143.145	-1112.264	-1118.383	150.791	24.762	146.147

# Appendix B (continued)

TABLE B2 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Ga (cr)	69.72300	-5.640	-5.640	0.000	26.099	5.640	41.220
GaBr3 (cr)	309.43500	-412.000	-369.580	-387.000	99.000	25.000	180.000
GaCl3 (cr)	176.08110	-547.000	-527.588	-527.000	96.000	20.000	134.000
GaF3 (cr)	126.71821	-1191.700	-1172.822	-1175.000	89.000	16.700	96.000
GaI3 (cr)	450.43641	-247.000	-221.566	-218.000	100.000	29.000	205.000
Ga2O3 (cr)	187.44420	-1105.550	-1081.250	-1091.000	92.131	14.550	84.940
Ge (cr)	72.61000	-4.636	-4.636	0.000	23.222	4.636	31.090
GeO2 (II)	104.60880	-587.430	-574.114	-580.200	50.166	7.230	39.710
GeS (cr)	104.67600	-85.005	-75.957	-75.348	47.782	9.657	66.480
GeS2 (II)	136.74200	-134.250	-120.790	-121.500	65.700	12.750	93.600
HBO2 (cr)	43.81774	-813.060	-798.932	-804.600	54.706	8.460	49.000
H2O (cr)	18.01528	(a)	(a)	-292.727	41.977	(a)	44.827
H2O (L)	18.01528	-299.108	-286.300	-285.830	75.351	13.278	69.942
H2SO4 (L)	98.07948	-842.215	-811.975	-813.989	138.584	28.226	156.895
H3BO3 (cr)	61.83302	-1108.320	-1081.384	-1094.800	86.060	13.520	89.950
H3PO4 (cr)	97.99518	-1301.468	-1266.046	-1284.488	106.064	16.980	110.544
Hg (cr)	200.59000	-9.343	-9.343	0.001	27.975	9.344	76.030
HgBr2 (cr)	360.39800	(a)	(a)	-175.310	75.312	(a)	170.314
HgO (cr)	216.58940	-99.893	-86.210	-90.789	44.062	9.104	70.270
I2 (cr)	253.80894	-13.196	-13.196	0.000	54.440	13.196	116.139
In (cr)	114.81800	-6.610	-6.610	0.000	26.900	6.610	57.651
InBr (cr)	194.72200	-187.200	-168.330	-175.000	50.000	12.200	110.000
InBr3 (cr)	354.53000	-423.500	-380.110	-399.000	102.000	24.500	175.000
InCl (crII)	150.27070	-198.900	-187.699	-186.500	51.460	12.400	100.000
InCl3 (cr)	221.17610	-551.000	-530.618	-530.000	100.000	21.000	142.000
InF3 (cr)	171.81321	-1209.400	-1189.552	-1190.000	91.999	19.400	110.000
InI (cr)	241.72247	-115.854	-102.646	-102.500	52.789	13.354	120.100
InI2 (crII)	368.62694	-195.197	-175.391	-176.000	77.320	19.197	173.900
InI3 (cr)	495.53141	-253.888	-227.484	-224.000	102.900	29.888	223.100
In2O3 (cr)	277.63420	-939.600	-913.360	-923.000	99.070	16.600	101.800
K (cr)	39.09830	-7.088	-7.088	0.000	29.600	7.088	64.680
KALO2 (II)	98.07864	-1143.955	-1123.647	-1130.600	76.120	13.355	85.550
KBO2 (cr)	81.90810	-995.114	-978.132	-983.000	67.030	12.114	80.000
KBr (cr)	119.00230	-405.660	-386.312	-393.450	52.470	12.210	95.920
KCN (II)	65.11574	-130.813	-118.336	-113.470	66.391	17.343	127.780
KCL (cr)	74.55100	-447.860	-436.181	-436.490	51.300	11.370	82.570
KF (cr)	58.09670	-579.900	-568.399	-569.900	48.990	10.000	66.500
KH (cr)	40.10624	-65.620	-54.298	-57.820	37.900	7.800	51.300
K (HF2) (a)	78.10305	-946.527	-926.380	-931.233	76.940	15.294	104.264
KI (cr)	166.00277	-342.000	-328.314	-329.300	52.800	12.700	106.050
KNO2 (II)	85.10384	-388.840	-368.737	-365.900	107.400	22.940	152.100
KNO3 (a)	101.10324	-512.750	-488.307	-494.000	95.060	18.750	132.900
KOH (a)	56.10564	-436.000	-420.338	-423.400	68.930	12.600	81.250
KOH (a)	56.10564	-436.000	-420.338	-423.400	68.930	12.600	81.250
KO2 (b)	71.09710	-300.420	-284.652	-283.600	77.530	16.820	125.400
K2CO3 (a)	138.20550	-1174.165	-1145.915	-1151.500	114.430	22.665	155.500
K2O (c)	94.19600	-375.400	-356.884	-361.700	72.000	13.700	96.000
K2O2 (cr)	110.19540	-460.000	-437.144	-443.000	91.000	17.000	117.000
K2S (cr)	110.26260	(a)	(a)	-376.560	74.684	(a)	115.060
K2SO4 (II)	174.26020	-1463.135	-1427.187	-1437.700	131.460	25.435	175.560
K2SiO3 (cr)	154.28030	-1564.860	-1534.446	-1543.000	117.570	21.860	146.000
K2Si2O5 (a)	214.36460	-2533.820	-2491.509	-2505.000	160.950	28.820	190.580
K3AlF6 (II)	258.26686	-3389.600	-3337.321	-3347.000	223.000	42.600	285.000
Li (cr)	6.94100	-4.632	-4.632	0.000	24.860	4.632	29.120
LiAlO2 (cr)	65.92134	-1198.369	-1180.517	-1188.674	67.777	9.694	53.313

# Appendix B (continued)

TABLE B2 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
LiBO <sub>2</sub> (cr)	49.75080	-1031.780	-1017.254	-1022.900	59.800	8.880	51.270
LiBr (cr)	86.84500	-361.636	-344.744	-351.160	49.830	10.476	74.010
LiCl (cr)	42.39370	-417.840	-408.617	-408.540	47.990	9.300	59.270
LiF (cr)	25.93940	-624.773	-615.728	-618.300	41.800	6.473	35.660
LiH (cr)	7.94894	-94.533	-85.667	-90.650	28.950	3.883	20.600
LiI (cr)	133.84547	-284.560	-273.330	-273.200	51.040	11.360	86.710
LiNO <sub>2</sub> (II)	52.94654	-380.400	-362.753	-368.300	63.000	12.100	88.000
LiNO <sub>3</sub> (cr)	68.94594	-495.500	-473.513	-482.700	89.000	12.800	104.000
LiOH (cr)	23.94834	-494.914	-481.708	-487.500	49.579	7.414	42.810
Li <sub>2</sub> CO <sub>3</sub> (cr)	73.89090	-1229.280	-1205.942	-1214.100	98.320	15.180	90.120
Li <sub>2</sub> O (cr)	29.88140	-605.131	-591.527	-597.880	54.100	7.251	37.610
Li <sub>2</sub> O <sub>2</sub> (cr)	45.88080	-643.000	-625.056	-632.500	75.000	10.500	58.000
Li <sub>2</sub> SO <sub>4</sub> (a)	109.94560	-1454.631	-1423.595	-1436.000	117.570	18.631	113.970
Li <sub>3</sub> AlF <sub>6</sub> (IV)	161.79496	-3421.750	-3376.839	-3389.600	202.530	32.150	187.900
Li <sub>3</sub> N (cr)	34.82974	-175.770	-157.539	-164.557	75.266	11.213	62.593
Mg (cr)	24.30500	-4.979	-4.979	0.000	24.775	4.979	32.535
MgAl <sub>2</sub> O <sub>4</sub> (cr)	142.26568	-2363.590	-2332.170	-2299.110	116.198	64.480	88.692
MgBr <sub>2</sub> (cr)	184.11300	-541.500	-512.001	-526.000	73.219	15.500	117.000
MgCO <sub>3</sub> (cr)	84.31390	-1107.630	-1088.578	-1096.000	76.108	11.631	65.090
MgCl <sub>2</sub> (cr)	95.21040	-658.070	-643.910	-644.300	71.384	13.770	89.620
MgF <sub>2</sub> (cr)	62.30181	-1134.120	-1120.316	-1124.200	61.587	9.920	57.200
MgH <sub>2</sub> (b)	26.32088	-81.010	-67.563	-75.700	35.350	5.310	31.100
MgI <sub>2</sub> (cr)	278.11394	-387.000	-368.825	-370.000	74.475	17.000	134.000
MgO (cr)	40.30440	-606.760	-597.441	-601.600	37.237	5.160	26.950
Mg(OH) <sub>2</sub> (cr)	58.31968	-935.760	-913.633	-924.350	77.111	11.410	63.180
MgS (cr)	56.37100	-356.330	-346.939	-348.000	45.560	8.330	50.330
MgSO <sub>4</sub> (II)	120.36860	-1304.200	-1277.449	-1288.800	96.399	15.400	91.600
MgSiO <sub>3</sub> (I)	100.38870	-1561.029	-1539.813	-1548.917	81.927	12.113	67.768
MgTiO <sub>3</sub> (cr)	120.17020	-1586.113	-1563.289	-1572.556	91.881	13.556	74.559
MgTi <sub>2</sub> O <sub>5</sub> (cr)	200.03600	-2530.658	-2494.330	-2508.219	146.858	22.439	135.603
Mg <sub>2</sub> SiO <sub>4</sub> (cr)	140.69310	-2194.358	-2163.822	-2177.078	118.688	17.280	95.140
Mg <sub>2</sub> TiO <sub>4</sub> (cr)	160.47460	-2183.191	-2151.048	-2164.354	128.574	18.836	115.102
Mg <sub>3</sub> N <sub>2</sub> (cr)	100.92848	-471.800	-448.193	-461.300	92.049	10.500	85.000
Mn (a)	54.93805	-4.994	-4.994	0.000	26.299	4.994	32.010
Mo (cr)	95.94000	-4.585	-4.585	0.000	23.933	4.585	28.605
MoO <sub>2</sub> (cr)	127.93880	-597.628	-584.363	-589.300	55.910	8.328	46.510
MoO <sub>3</sub> (cr)	143.93820	-757.190	-739.585	-744.600	75.070	12.590	77.660
NH <sub>4</sub> Cl (II)	53.49120	-337.251	-311.389	-314.553	86.441	22.698	94.860
NH <sub>4</sub> F (cr)	37.03690	-478.668	-452.984	-467.560	65.269	11.108	71.970
Na (cr)	22.98977	-6.460	-6.460	0.000	28.230	6.460	51.300
NaAlO <sub>2</sub> (a)	81.97011	-1156.984	-1137.304	-1133.190	73.638	23.794	70.400
NaBO <sub>2</sub> (cr)	65.79957	-988.132	-971.778	-976.500	65.940	11.632	73.530
NaBr (cr)	102.89377	-372.750	-354.030	-361.160	51.380	11.590	86.930
NaCN (II)	49.00721	-110.131	-98.283	-90.709	69.036	19.422	118.457
NaCl (cr)	58.44247	-421.860	-410.809	-411.260	50.500	10.600	72.150
NaF (cr)	41.98817	-585.082	-574.209	-576.600	46.820	8.482	51.160
NaH (cr)	23.99771	-62.639	-51.945	-56.380	36.400	6.259	40.000
NaI (cr)	149.89424	-301.890	-288.832	-289.630	52.090	12.260	98.560
NaNO <sub>2</sub> (I)	68.99531	-371.100	-351.625	-354.600	69.000	16.500	106.000
NaNO <sub>3</sub> (a)	84.99471	-484.930	-461.115	-467.700	93.050	17.230	116.400
NaOH (a)	39.99711	-436.290	-421.256	-425.800	59.530	10.490	64.430
NaO <sub>2</sub> (cr)	54.98857	-279.300	-264.160	-261.000	72.130	18.300	115.900
Na <sub>2</sub> CO <sub>3</sub> (a)	105.98844	-1149.940	-1122.946	-1129.190	112.300	20.750	135.000
Na <sub>2</sub> O (c)	61.97894	-426.970	-409.710	-414.570	69.120	12.400	75.040
Na <sub>2</sub> O <sub>2</sub> (b)	77.97834	-527.694	-506.094	-512.000	89.330	15.694	94.770

# Appendix B (continued)

TABLE B2 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
Na2S (cr)	78.04554	(a)	(a)	-366.100	82.801	(a)	96.232
Na2SO3 (cr)	126.04374	(a)	(a)	-1100.802	120.247	(a)	145.938
Na2SO4 (V)	142.04314	-1411.104	-1376.412	-1387.900	128.040	23.204	149.580
Na3ALF6 (a)	209.94127	-3360.470	-3310.075	-3322.400	215.900	38.070	238.200
Na5AL3F14 (cr)	461.87111	-7635.830	-7528.134	-7555.000	454.000	80.830	515.200
Nb (cr)	92.90638	-5.241	-5.241	0.000	24.694	5.241	36.464
NbO (cr)	108.90578	-413.200	-403.619	-406.000	41.000	7.200	46.000
NbOCL3 (cr)	215.26388	(a)	(a)	-879.500	119.820	(a)	142.000
NbO2 (II)	124.90518	-804.267	-790.346	-795.000	57.660	9.267	54.290
Nb2O5 (cr)	265.80976	-1919.240	-1887.058	-1897.000	131.950	22.240	137.100
Ni (cr)	58.69340	-4.786	-4.786	0.000	25.987	4.786	29.870
NiS (b)	90.75940	-96.329	-87.131	-87.864	47.112	8.465	52.992
NiS2 (cr)	122.82540	(a)	(a)	-131.378	70.626	(a)	71.965
Ni3S2 (a)	240.21220	-239.142	-215.960	-217.986	117.654	21.156	133.888
Ni3S4 (cr)	304.34420	(a)	(a)	-301.115	164.808	(a)	186.481
P (cr)	30.97376	-5.360	-5.360	0.000	23.824	5.360	41.090
P4O10 (cr)	283.88904	-3044.320	-2979.479	-3010.100	215.569	34.220	231.000
Pb (cr)	207.20000	-6.870	-6.870	0.000	26.650	6.870	64.800
PbBr2 (cr)	367.00800	-295.930	-264.540	-276.700	79.580	19.230	161.100
PbCL2 (cr)	278.10540	-376.550	-360.499	-359.400	76.985	17.150	136.000
PbF2 (II)	245.19681	-691.000	-675.305	-676.000	72.259	15.000	106.000
PbI2 (cr)	461.00894	-195.500	-175.434	-176.000	77.570	19.500	174.850
PbO (II-r)	223.19940	-227.825	-216.615	-218.600	46.414	9.225	67.840
PbO2 (cr)	239.19880	-286.962	-271.412	-276.000	60.997	10.962	71.920
PbS (cr)	239.26600	-110.985	-99.703	-99.475	49.499	11.510	91.200
Pb2O3 (cr)	462.39820	-512.580	-485.820	-491.700	107.701	20.880	151.900
Pb3O4 (cr)	685.59760	-749.830	-711.860	-720.000	146.705	29.830	211.300
Rb (cr)	85.46780	-7.489	-7.489	0.000	31.060	7.489	76.780
RbBO2 (b)	128.27760	-988.310	-970.927	-975.000	73.390	13.310	94.320
RbBr (cr)	165.37180	-407.830	-388.081	-394.770	52.760	13.060	110.100
RbCL (cr)	120.92050	-447.380	-435.300	-435.220	52.260	12.160	95.230
RbF (cr)	104.46620	-570.600	-558.698	-559.700	50.630	10.900	77.700
RbH (cr)	86.47574	-61.400	-49.677	-52.300	39.300	9.100	63.700
RbI (cr)	212.37227	-346.940	-332.853	-333.600	52.590	13.340	118.800
RbNO2 (I)	131.47334	-390.400	-369.896	-367.000	84.000	23.400	162.000
RbNO3 (IV)	147.47274	-514.340	-489.496	-494.700	99.000	19.640	144.900
RbOH (b)	102.47514	-432.300	-416.237	-418.800	69.000	13.500	94.000
RbO2 (b)	117.46660	-295.860	-279.691	-279.100	77.570	16.760	130.100
Rb2CO3 (a)	230.94450	-1157.080	-1128.028	-1132.600	117.600	24.480	181.330
Rb2O (c)	186.93500	-353.600	-334.282	-338.000	74.000	15.600	125.000
Rb2O2 (b)	202.93440	-429.700	-406.042	-410.000	93.000	19.700	160.000
Rb2SO4 (a)	266.99920	-1462.914	-1426.164	-1435.900	134.055	27.014	197.500
S (a)	32.06600	-4.412	-4.412	0.000	22.690	4.412	32.070
SCL2 (L)	102.97140	(a)	(a)	-49.790	91.002	(a)	183.678
S2CL2 (L)	135.03740	(a)	(a)	-58.158	124.290	(a)	223.844
Sc (a)	44.95591	-5.207	-5.207	0.000	25.510	5.207	34.770
Sc2O3 (cr)	137.91002	-1922.530	-1899.096	-1908.600	94.220	13.930	76.800
Si (cr)	28.08550	-3.217	-3.217	0.000	19.789	3.217	18.810
SiC (b)	40.09620	-76.272	-72.001	-73.000	26.860	3.272	16.610
SiO2 (a-qz)	60.08430	-917.616	-905.718	-910.700	44.602	6.916	41.460
SiS (cr)	60.15150	-177.738	-170.108	-168.737	45.000	9.000	63.000
SiS2 (cr)	92.21750	-298.180	-286.139	-287.000	61.630	11.180	76.860
Si2N2O (cr)	100.18388	(a)	(a)	-947.700	65.560	(a)	45.350
Si3N4 (cr)	140.28346	-799.913	-772.921	-787.800	93.010	12.113	66.065
Sn (cr)	118.71000	-6.323	-6.323	0.000	27.112	6.323	51.180

# Appendix B (continued)

TABLE B2 (continued)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$T = 298.15 \text{ K}$			
				$\Delta_f H^{\circ}(T)$ kJ/mol	$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
SnBr2 (cr)	278.51800	-272.270	-241.427	-253.600	78.970	18.670	153.000
SnBr4 (cr)	438.32600	-419.260	-363.897	-388.000	133.300	31.260	260.000
SnCL2 (cr)	189.61540	-350.330	-334.826	-333.000	78.051	17.330	134.100
SnCL4 (L)	260.52080	-555.740	-531.055	-517.000	157.400	38.740	265.000
SnF2 (cr)	156.70681	-691.200	-676.052	-677.000	72.395	14.200	96.200
SnI2 (cr)	372.51894	-171.950	-152.431	-153.000	78.310	18.950	168.500
SnI4 (cr)	626.32788	-239.100	-206.385	-207.500	131.550	31.600	282.700
SnO (cr)	134.70940	-289.446	-278.783	-280.710	47.783	8.736	57.170
SnO2 (cr)	150.70880	-586.014	-571.011	-577.630	53.219	8.384	49.010
SnS (cr)	150.77600	-120.192	-109.457	-109.662	49.245	10.530	77.000
SnS2 (cr)	182.84200	-155.147	-140.000	-141.837	70.123	13.310	87.400
Sr (a)	87.62000	-6.558	-6.558	0.000	26.830	6.558	54.999
SrBr2 (a)	247.42800	-740.060	-708.982	-722.000	76.527	18.060	143.440
SrCO3 (a)	147.62890	-1241.120	-1220.489	-1226.000	82.424	15.121	97.200
SrCL2 (a)	158.52540	-849.230	-833.491	-833.000	75.605	16.230	114.850
SrF2 (a)	125.61681	-1242.075	-1226.692	-1229.000	70.000	13.075	82.130
SrH2 (a)	89.63588	-188.000	-172.974	-180.000	44.000	8.000	52.000
SrI2 (cr)	341.42894	-586.920	-567.166	-568.000	77.404	18.920	159.100
SrO (cr)	103.61940	-599.680	-588.782	-591.000	45.250	8.680	55.580
Sr (OH) 2 (b)	121.63468	-979.572	-955.866	-964.300	89.220	15.272	94.990
SrS (cr)	119.68600	-490.040	-479.070	-480.000	48.700	10.041	68.200
SrSO4 (a)	183.68360	-1475.400	-1447.070	-1457.000	102.000	18.400	121.000
Ta (cr)	180.94790	-5.681	-5.681	0.000	25.295	5.681	41.471
TaC (cr)	192.95860	-150.611	-143.877	-144.097	36.790	6.514	42.371
Ta2O5 (II)	441.89280	-2071.950	-2038.888	-2049.000	134.935	22.950	141.900
Th (a)	232.03810	-6.350	-6.350	0.000	26.230	6.350	51.830
Ti (a)	47.86700	-4.824	-4.824	0.000	25.060	4.824	30.720
TiB (cr)	58.67800	(a)	(a)	-160.247	29.673	(a)	34.727
TiB2 (cr)	69.48900	-285.068	-277.816	-279.491	44.279	5.577	28.485
TiC (cr)	59.87770	-188.703	-182.825	-184.096	33.807	4.607	24.230
TiCL2 (cr)	118.77240	-528.771	-514.766	-515.470	69.831	13.301	87.345
TiCL3 (cr)	154.22510	-742.660	-724.064	-721.740	97.161	20.920	139.750
TiCL4 (L)	189.67780	-831.128	-807.942	-804.165	145.205	26.963	252.379
TiN (cr)	61.87374	-343.136	-333.977	-337.649	37.079	5.487	30.234
TiO (a)	63.86640	-548.175	-539.011	-542.000	39.905	6.175	34.790
TiO2 (cr)	79.86580	-952.680	-939.176	-944.000	55.080	8.680	50.620
Ti2O3 (I)	143.73220	-1534.090	-1511.422	-1520.000	95.810	14.090	77.290
Ti3O5 (a)	223.59800	-2479.630	-2443.458	-2457.000	150.830	22.630	126.200
Ti4O7 (cr)	303.46380	-3438.630	-3388.954	-3403.000	216.810	35.630	201.480
U (a)	238.02890	-6.364	-6.364	0.000	27.665	6.364	50.200
UF3 (cr)	295.02411	-1527.080	-1507.478	-1508.700	95.100	18.380	123.400
UF4 (cr)	314.02251	-1943.050	-1919.036	-1920.500	116.020	22.550	151.670
UF5 (b)	333.02092	-2109.150	-2080.723	-2083.000	132.000	26.150	179.500
UF6 (cr)	352.01932	-2229.265	-2196.426	-2197.700	166.750	31.565	227.800
UO2 (cr)	270.02770	-1096.280	-1081.236	-1085.000	63.600	11.280	77.030
UO2F2 (cr)	308.02451	-1673.300	-1649.431	-1653.600	103.200	19.700	135.500
UO3 (c)	286.02710	-1238.385	-1219.001	-1223.800	81.670	14.585	96.110
U3O8 (II)	842.08190	-3617.540	-3563.728	-3574.800	238.338	42.740	282.549
U4O9 (III)	1096.11020	-4562.750	-4498.234	-4512.000	293.340	50.750	334.130
V (cr)	50.94150	-4.640	-4.640	0.000	24.896	4.640	28.936
VCL2 (cr)	121.84690	(a)	(a)	-451.872	71.868	(a)	97.069
VCL3 (cr)	157.29960	(a)	(a)	-581.116	93.174	(a)	130.959
VN (cr)	64.94824	-223.376	-214.401	-217.150	37.982	6.226	37.263
VO (cr)	66.94090	-436.780	-427.800	-430.800	38.420	5.980	33.510
V2O3 (cr)	149.88120	-1233.930	-1211.630	-1216.800	100.960	17.130	94.490

# Appendix B (continued)

TABLE B2 (concluded)

Species name	Molecular weight	$H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(0)$ kJ/mol	$\Delta_f H^{\circ}(T)$ kJ/mol	$T = 298.15 \text{ K}$		
					$C_p^{\circ}(T)$ J/K-mol	$H^{\circ}(T) - H^{\circ}(0)$ kJ/mol	$S^{\circ}(T)$ J/K-mol
V2O4 (II)	165.88060	-1449.320	-1422.680	-1432.600	112.130	16.720	93.180
V2O5 (cr)	181.88000	-1572.210	-1541.230	-1551.000	127.770	21.210	130.500
W (cr)	183.84000	-4.973	-4.973	0.000	24.295	4.973	32.660
WC (cr)	195.85070	(a)	(a)	-40.540	35.378	(a)	32.384
WCL6 (I)	396.55620	(a)	(a)	-593.710	175.418	(a)	238.488
WOCL4 (cr)	341.65020	(a)	(a)	-671.114	146.248	(a)	172.799
WO2 (cr)	215.83880	-596.811	-583.158	-588.100	55.780	8.711	50.640
WO2CL2 (cr)	286.74420	(a)	(a)	-780.316	104.408	(a)	200.832
WO3 (III)	231.83820	-854.580	-836.587	-841.300	79.705	13.280	81.640
Zn (cr)	65.39000	-5.657	-5.657	0.000	25.390	5.657	41.630
ZnSO4 (a)	161.45360	-997.382	-969.953	-980.144	99.035	17.238	110.541
Zr (a)	91.22400	-5.497	-5.497	0.000	25.202	5.497	38.869
ZrC (cr)	103.23470	-202.510	-195.959	-196.648	37.899	5.862	33.321
ZrN (cr)	105.23074	-377.828	-367.996	-371.238	40.443	6.590	38.861
ZrO2 (III)	123.22280	-1109.051	-1094.874	-1100.300	55.920	8.751	50.390
CH3OH (L)	32.04186	-257.905	-235.575	-238.910	81.080	18.995	127.270
C2H5OH (L)	46.06844	-301.592	-269.741	-277.510	112.250	24.082	160.100
C6H6 (L)	78.11184	18.970	50.695	49.080	135.950	30.110	173.440
C6H5NH2 (L)	93.12652	-2.520	37.774	31.500	191.920	34.020	191.060
C6H14 (L), n-hexa	86.17536	-245.580	-179.982	-198.660	195.480	46.920	296.090
C7H8 (L)	92.13842	-21.290	19.957	12.180	157.290	33.470	221.030
C7H16 (L), n-hept	100.20194	-276.990	-201.871	-224.350	224.980	52.640	328.560
C8H18 (L), n-octa	114.22852	-311.750	-227.109	-250.260	254.150	61.490	361.070
C8H18 (L), isooct	114.22852	-309.350	-224.709	-259.160	239.000	50.190	328.110
H2O2 (L)	34.01468	-210.729	-193.581	-187.780	89.330	22.949	109.602
Jet-A (L)	167.31102	(a)	(a)	-303.403	350.332	(a)	448.106
NH4CLO4 (I)	117.48880	-321.005	-277.783	-295.767	128.072	25.238	184.180
NH4NO3 (IV)	80.04344	-389.262	-350.636	-365.600	139.080	23.662	150.810
N2H4 (L)	32.04524	(a)	(a)	50.380	98.840	(a)	121.544

<sup>a</sup>No data available for 0 K.

## Appendix B (continued)

**TABLE B3.—ASSIGNED ENTHALPIES FOR SPECIES THAT ARE USED IN CEA AS REACTANTS ONLY**

Species name	Phase	Stoichiometry								Molecular weight	$H^{\circ}(T)$	$T$ K
Air	gas	<sup>a</sup> N	1.56	O	0.42	Ar	0.01	C	0.00	28.96518	-0.126	298.15
B2H6 (L)	liq	B	2.00	H	6.00				0.00	27.66964	16.445	180.59
B5H9 (L)	liq	B	5.00	H	9.00				0.00	63.12646	42.840	298.15
(CH2)x(cr)	sol	C	1.00	H	2.00				0.00	14.02658	-25.600	298.15
CH3NO2 (L)	liq	C	1.00	H	3.00	N	1.00	O	2.00	61.04006	-113.100	298.15
CH4 (L)	liq	C	1.00	H	4.00				0.00	16.04246	-89.233	111.64
CH3OH (L)	liq	C	1.00	H	4.00	O	1.00		0.00	32.04186	-238.910	298.15
CH6N2 (L)	liq	C	1.00	H	6.00	N	2.00		0.00	46.07182	54.200	298.15
C2H2 (L), acetylene	liq	C	2.00	H	2.00				0.00	26.03728	207.599	192.35
CH3CN (L)	liq	C	2.00	H	3.00	N	1.00		0.00	41.05196	31.380	298.15
C2H4 (L)	liq	C	2.00	H	4.00				0.00	28.05316	33.945	169.42
C2H4O (L), ethylene	liq	C	2.00	H	4.00	O	1.00		0.00	44.05256	-78.841	283.65
C2H6 (L)	liq	C	2.00	H	6.00				0.00	30.06904	-103.819	184.56
C2H5OH (L)	liq	C	2.00	H	6.00	O	1.00		0.00	46.06844	-277.510	298.15
C2H8N2 (L), UDMH	liq	C	2.00	H	8.00	N	2.00		0.00	60.09840	48.900	298.15
C2N2 (L)	liq	C	2.00	N	2.00				0.00	52.03488	283.209	252.05
C3H6 (L), propylene	liq	C	3.00	H	6.00				0.00	42.07974	-2.704	225.46
C3H7NO3 (L)	liq	C	3.00	H	7.00	N	1.00	O	3.00	105.09262	-214.500	298.15
C3H8 (L)	liq	C	3.00	H	8.00				0.00	44.09562	-128.228	231.08
C4H8 (L), 1-butene	liq	C	4.00	H	8.00				0.00	56.10632	-25.173	266.92
C4H10 (L), n-butane	liq	C	4.00	H	10.00				0.00	58.12220	-150.664	272.64
C4H10 (L), isobutane	liq	C	4.00	H	10.00				0.00	58.12220	-159.664	261.36
C5H12 (L), n-pentane	liq	C	5.00	H	12.00				0.00	72.14878	-173.490	298.15
C6H6 (L)	liq	C	6.00	H	6.00				0.00	78.11184	49.080	298.15
C6H5NH2 (L)	liq	C	6.00	H	7.00	N	1.00		0.00	93.12652	31.500	298.15
C6H14 (L), n-hexane	liq	C	6.00	H	14.00				0.00	86.17536	-198.660	298.15
C7H8 (L)	liq	C	7.00	H	8.00				0.00	92.13842	12.180	298.15
C7H16 (L), n-heptane	liq	C	7.00	H	16.00				0.00	100.20194	-224.350	298.15
C8H18 (L), n-octane	liq	C	8.00	H	18.00				0.00	114.22852	-250.260	298.15
C8H18 (L), isooctane	liq	C	8.00	H	18.00				0.00	114.22852	-259.160	298.15
CLF3 (L)	liq	CL	1.00	F	3.00				0.00	92.44791	-193.386	284.89
CLO3F	gas	CL	1.00	O	3.00	F	1.00		0.00	102.44930	-23.800	298.15
CLO3F (L)	liq	CL	1.00	O	3.00	F	1.00		0.00	102.44930	-47.436	226.40
CL2 (L)	liq	CL	2.00		0.00				0.00	70.90540	-22.550	239.12
F2 (L)	liq	F	2.00		0.00				0.00	37.99681	-13.091	85.02
F2O (L)	liq	F	2.00	O	1.00				0.00	53.99621	6.672	128.40
HNO3 (L)	liq	H	1.00	N	1.00	O	3.00		0.00	63.01288	-173.013	298.15
H2 (L)	liq	H	2.00		0.00				0.00	2.01588	-9.012	20.27
H2O2 (L)	liq	H	2.00	O	2.00				0.00	34.01468	-187.780	298.15
IRFNA	liq	H	1.57	N	1.63	O	4.70	F	0.02	100.00000	-270.496	298.15
JP-4	liq	C	1.00	H	1.94				0.00	13.96842	-22.723	298.15
JP-5	liq	C	1.00	H	1.92				0.00	13.94443	-22.183	298.15
JP-10 (L)	liq	C	10.00	H	16.00				0.00	136.23404	-122.800	298.15
JP-10 (g)	gas	C	10.00	H	16.00				0.00	136.23404	-86.856	298.15
Jet-A (L)	liq	C	12.00	H	23.00				0.00	167.31102	-303.403	298.15
Jet-A (g)	gas	C	12.00	H	23.00				0.00	167.31102	-249.657	298.15
LiCLO4 (cr)	sol	LI	1.00	CL	1.00	O	4.00		0.00	106.39130	-380.700	298.15
NF3 (L)	liq	N	1.00	F	3.00				0.00	71.00195	-150.387	144.09
NH3 (L)	liq	N	1.00	H	3.00				0.00	17.03056	-71.555	239.72
NH4CLO4 (I)	liq	N	1.00	H	4.00	CL	1.00	O	4.00	117.48880	-295.767	298.15

<sup>a</sup>Stoichiometry for air: N, 1.56168; O, 0.419590; Ar, 0.009365; C, 0.000319.



## Appendix B (*concluded*)

TABLE B3 (*concluded*)

Species name	Phase	Stoichiometry							Molecular weight	$H^o(T)$	$T$ K
NH <sub>4</sub> NO <sub>3</sub> (I)	liq	N	2.00	H	4.00	O	3.00	0.00	80.04344	-365.600	298.15
N <sub>2</sub> (L)	liq	N	2.00		0.00		0.00	0.00	28.01348	-12.107	77.35
N <sub>2</sub> H <sub>4</sub> (L)	liq	N	2.00	H	4.00		0.00	0.00	32.04524	50.380	298.15
N <sub>2</sub> O <sub>4</sub> (L)	liq	N	2.00	O	4.00		0.00	0.00	92.01108	-17.549	298.15
O <sub>2</sub> (L)	liq	O	2.00		0.00		0.00	0.00	31.99880	-12.979	90.17
O <sub>3</sub> (L)	liq	O	3.00		0.00		0.00	0.00	47.99820	122.527	161.85
RP-1	liq	C	1.00	H	1.95		0.00	0.00	13.97820	-24.717	298.15



## Appendix C

### Format for Thermodynamic Data Coefficients

This appendix explains the format for data contained in the file thermo.inp (app. D). Equations (1) to (3) are repeated here for convenience:

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

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

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

**TABLE C1.—FORTRAN FORMAT USED FOR DATA IN APPENDIX D**

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

<sup>a</sup> Condensed phases are numbered in increasing order by temperature.

For example, the following data are for condensed titanium nitride:

```

1234567890123456789012345678901234567890123456789012345678901234567890
      10          20          30          40          50          60          70          80

1  TiN(cr)           Chase,1998 pp1612-4.
2  2 j 6/68 TI  1.00N  1.00  0.00  0.00  0.00  0.00  1  61.87374  -337648.800
3  200.000  800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0  5487.000
4  -5.479117220D+05 9.328691110D+03-6.386263890D+01 2.429925456D-01-4.304234520D-04
5  3.792645100D-07-1.317412256D-10 -8.424256140D+04 3.392988560D+02
6  800.000  3220.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0  5487.000
7  -3.656247060D+05 1.265730431D+03 3.831711190D+00 1.632900455D-03-1.062786626D-07
8  1.310931390D-11-5.770548410D-16 -5.027654400D+04-1.652632899D+01
9  TiN(L)           Chase,1998 pp1612-4.
10 1 j 6/68 TI  1.00N  1.00  0.00  0.00  0.00  0.00  2  61.87374  -337648.800
11 3220.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0  5487.000
12 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00
13 0.000000000D+00 0.000000000D+00 -3.626039860D+04-3.958296649D+01

```

## Appendix C (concluded)

There are two sets of data: one for the crystal and one for the liquid. We focus first on the crystalline phase (records 1 to 8): record 1 lists the name as TiN(cr) and tells us that the data for this phase originated from Chase (1998), pp. 1612–1614. Record 2 gives the following information:

**TABLE C2.—EXPLANATION OF SECOND RECORD FOR TiN(cr) DATA**

Columns	Contents	Explanation
2	2	Number of intervals covered by the data
4 to 9	j 6/68	Internal NASA reference code (see app. D)
11 to 26	TI 1.00N 1.00	Molecular formula [unused places (11 to 50) filled with blanks and zeros]
52	1	(First) condensed phase
58 to 65	61.87374	Molecular weight
70 to 80	–337648.800	$\Delta_f H^\circ(298.15)$ in J/mol

Records 3 to 5 cover the temperature interval 200 to 800 K. The single digit “7” after the temperature range says that  $C_p^\circ(T)/R$  is described by seven coefficients in each interval. The next eight 5-place fields on record 3 list the temperature exponents in the empirical equation for  $C_p^\circ(T)/R$  used in this temperature interval. The last entry on record 3 contains a value of 5487.00 J/mol for  $H^\circ(298.15) - H^\circ(0)$ . This field will contain the number 0.0000 if  $H^\circ(298.15) - H^\circ(0)$  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 to 8 contain these coefficients for the temperature range 800 to 3220 K. Both intervals use equation (1) to describe  $C_p^\circ(T)/R$ .

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

## Appendix D

### Listing of NASA Glenn Thermodynamic Data Coefficients

The remainder of this appendix is a listing of the data file “thermo.inp,” which is the subject of this report. The initial lines that start with an exclamation point are comments. See the text and Appendix C for a further explanation of these data.

```

!           SIX-CHARACTER REFERENCE-DATE CODES
!
!  Letters      Reference      Numbers
!  -----
!  j           NIST-JANAF Thermochemical      Month/year of table
!             Tables. Chase,1998
!
!  tpis        Thermodynamic Properties of      Year of volume
!             Individual Substances. Gurvich,
!             1978,1979,1982,1989,1991,1996
!
!  n           TRC Thermodynamic Tables, NIST      Month/year of table
!
!  bar         Barin: Thermochemical Data of      Year of volume
!             Pure Substances. Barin,1989
!
!  coda        CODATA Key Values for      Year of volume
!             Thermodynamics. Cox,1989
!
!  srd         Standard Reference Data      Year of J. Phys. Chem. Ref.
!             Data journal
!
!           ORDER OF SPECIES
!
1)  Gaseous products/reactants, pages 45-210
2)  Condensed products/reactants, pages 210-276
3)  Gaseous/condensed reactants only, pages 276-280

thermo
  200.00  1000.00  6000.00  20000.    3/19/02
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
Ag      Hf:Cox,1989. Moore,1971. Gordon,1999.
3 g10/97 AG  1.00  0.00  0.00  0.00  0.00  0  107.8682000  284900.000
  200.000  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0  6197.428
0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
0.000000000D+00 0.000000000D+00 3.352002370D+04 6.562819350D+00
  1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0  6197.428
-3.309926370D+05 9.820086420D+02 1.381179917D+00 6.170899990D-04-1.688114600D-07
  2.008826848D-11-5.627285655D-16 2.726719171D+04 1.456862733D+01
  6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0  6197.428
-3.717441500D+08 2.758069172D+05-7.385982610D+01 9.606158720D-03-5.393935740D-07
  1.358856730D-11-1.272610104D-16 -2.107724971D+06 6.628374570D+02

```

## Appendix D (continued)

Ag+ Moore,1971. Gordon,1999.

3 g10/97 AG	1.00E	-1.00	0.00	0.00	0.00	0	107.8676514	1022093.730
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.691132750D+06	-4.316983000D+04	2.028445385D+02	-4.658413740D-01	5.586200510D-04				
-3.154880975D-07	6.578702060D-11		3.371574470D+05	-1.142924427D+03				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.327432350D+07	1.310710631D+05	-1.098820208D+02	4.826002760D-02	-1.093661557D-05				
1.263835910D-09	-5.852542535D-14		-7.439122510D+05	8.446266190D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.119469170D+08	1.159621936D+05	-2.220792532D+01	2.938747589D-03	-1.822389545D-07				
5.823925360D-12	-7.455184012D-17		-8.068014150D+05	2.271702823D+02				

Ag- Hotop,1985. Gordon,1999.

3 g10/97 AG	1.00E	1.00	0.00	0.00	0.00	0	107.8687486	153078.728
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		1.766565919D+04	5.869679800D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		1.766565919D+04	5.869679800D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		1.766565919D+04	5.869679800D+00				

AL Hf:Cox,1989. Kaufman,1991b. Gordon,1999.

3 g12/97 AL	1.00	0.00	0.00	0.00	0.00	0	26.9815380	330000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.006608890D+03	1.861304407D+01	2.412531111D+00	1.987604647D-04	-2.432362152D-07				
1.538281506D-10	-3.944375734D-14		3.887412680D+04	6.086585765D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.920820938D+04	1.167751876D+02	2.356906505D+00	7.737231520D-05	-1.529455262D-08				
-9.971670260D-13	5.053278264D-16		3.823288650D+04	6.600920155D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.040682320D+08	3.802322650D+05	-1.082347159D+02	1.549444292D-02	-1.070103856D-06				
3.592110900D-11	-4.696039394D-16		-2.901050501D+06	9.491883160D+02				

AL+ Kaufman,1991b. Moore,1971. Gordon,1999.

3 g 1/98 AL	1.00E	-1.00	0.00	0.00	0.00	0	26.9809894	913015.128
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		1.090644788D+05	3.791005780D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.181183250D+03	-9.948557270D+00	2.548615878D+00	-5.878760040D-05	3.132291294D-08				
-7.748894630D-12	7.274447690D-16		1.091011485D+05	3.488667290D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.080958540D+08	5.509673040D+05	-1.279244177D+02	1.510503026D-02	-8.932051950D-07				
2.719381070D-11	-3.367986284D-16		-4.268693020D+06	1.141245444D+03				

AL- Chase,1998 p65 6/83. EA:Hotop,1985. Gordon,1999.

3 g 3/97 AL	1.00E	1.00	0.00	0.00	0.00	0	26.9820866	281090.113
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.910801723D+04	-3.836983750D+02	4.655142800D+00	-6.045821840D-03	8.577259640D-06				
-5.476260000D-09	1.322714061D-12		3.490616980D+04	-5.957097700D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.339814320D+05	-2.383438463D+03	5.469971130D+00	-1.299840355D-03	2.888305470D-07				
-3.253240510D-11	1.472436088D-15		4.780306540D+04	-1.536906816D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.901212850D+06	-2.296000877D+03	3.072774844D+00	-6.894714790D-05	4.413313240D-09				
-1.445353715D-13	1.905752608D-18		5.241871250D+04	1.451781383D+00				

ALBr Gurvich,1996a pt1 p184 pt2 p148.

2 tpis96 AL	1.00BR	1.00	0.00	0.00	0.00	0	106.8855380	14325.015
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.176158640D+03	-2.516942718D+02	5.403296330D+00	-1.747212920D-03	2.077304770D-06				
-1.261267579D-09	3.166335970D-13		1.635024429D+03	-2.323594886D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.103395600D+05	2.010066834D+03	1.769617961D+00	1.929888914D-03	-6.641047830D-07				
1.172854627D-10	-7.178742760D-15		-1.217812867D+04	2.204450764D+01				

ALBr2 Gurvich,1996a pt1 p186 pt2 p149.

2 tpis96 AL	1.00BR	2.00	0.00	0.00	0.00	0	186.7895380	-140662.125
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.199375870D+04	-7.119178970D+02	9.478258110D+00	-4.875531670D-03	5.516512990D-06				
-3.340053040D-09	8.368476840D-13		-1.540591306D+04	-1.742171366D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.523782900D+05	4.671544170D+02	7.111908190D+00	-5.551709200D-04	3.166301130D-07				
-5.521028330D-11	3.176725950D-15		-2.265004078D+04	-2.695610360D+00				

## Appendix D (continued)

ALBr3 Gurvich,1996a pt1 p188 pt2 p151.  
 2 tps96 AL 1.00BR 3.00 0.00 0.00 0.00 0 266.6935380 -410476.664  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17943.336  
 4.718948840D+04-1.053853163D+03 1.350747168D+01-6.639869930D-03 7.269276830D-06  
 -4.278049490D-09 1.045573281D-12 -4.699440330D+04-3.667936780D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17943.336  
 -8.935527440D+04-2.678035134D+01 1.002063997D+01-8.458764400D-06 1.904243317D-09  
 -2.215195785D-13 1.038219389D-17 -5.249247640D+04-1.579666403D+01

ALC Gurvich,1996a pt1 p205 pt2 p165.  
 2 tps96 AL 1.00C 1.00 0.00 0.00 0.00 0 38.9922380 682283.509  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9058.109  
 4.139921880D+04-5.858677890D+02 5.962445720D+00-2.006064322D-03 1.665566136D-06  
 -7.121649210D-10 1.271188744D-13 8.383436110D+04-8.002165050D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9058.109  
 1.937001487D+06-6.749117790D+03 1.347525643D+01-5.850802650D-03 1.926461091D-06  
 -2.585922351D-10 1.222659806D-14 1.225363649D+05-6.152244872D+01

ALC2 Gurvich,1996a pt1 p206 pt2 p166.  
 2 tps96 AL 1.00C 2.00 0.00 0.00 0.00 0 51.0029380 675615.776  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12262.776  
 1.524087465D+04-2.649987059D+02 6.280414900D+00-1.786037647D-04 3.791907740D-06  
 -3.999450070D-09 1.299752388D-12 8.092763280D+04-6.247291862D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12262.776  
 1.466017895D+05-1.362764489D+03 8.457759150D+00-3.678901680D-04 7.903174500D-08  
 -8.880023720D-12 4.053633950D-16 8.705924230D+04-2.127956728D+01

ALCL Gurvich,1996a pt1 p168 pt2 p131.  
 2 tps96 AL 1.00CL 1.00 0.00 0.00 0.00 0 62.4345380 -51007.443  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9323.112  
 2.380881392D+04-4.457159420D+02 5.992853990D+00-2.777300261D-03 3.101582418D-06  
 -1.815268376D-09 4.414662340D-13 -5.202736030D+03-7.383298016D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9323.112  
 -8.993461220D+05 2.765942061D+03 1.003500696D+00 2.267806833D-03-7.280541600D-07  
 1.182380673D-10 6.660498130D-15 -2.496164448D+04 2.616925480D+01

ALCL+ Chase,1998 p73.  
 2 j 6/76 AL 1.00CL 1.00E -1.00 0.00 0.00 0 62.4339894 861849.307  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9154.435  
 3.469955220D+04-5.479900030D+02 6.106011130D+00-2.674711519D-03 2.696426573D-06  
 -1.463885068D-09 3.358729060D-13 1.051719510D+05-7.816586372D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9154.435  
 -7.547240820D+05 1.251545253D+03 4.442424910D+00-9.786116430D-04 6.347511330D-07  
 -1.158320344D-10 6.870022460D-15 9.318332700D+04 4.047521108D+00

ALCL2 Gurvich,1996a pt1 p171 pt2 p132.  
 2 tps96 AL 1.00CL 2.00 0.00 0.00 0.00 0 97.8875380 -240874.252  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12846.859  
 5.340545950D+04-9.678057980D+02 1.006252671D+01-5.539528450D-03 5.823420560D-06  
 -3.306542450D-09 7.831562100D-13 -2.607627110D+04-2.393364216D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12846.859  
 4.303453060D+05-1.552370585D+03 8.760657420D+00-9.467450060D-04 2.401844880D-07  
 -2.427836709D-11 8.390123470D-16 -2.145884709D+04-1.803641668D+01

ALCL3 Gurvich,1996a pt1 p173 pt2 p134.  
 2 tps96 AL 1.00CL 3.00 0.00 0.00 0.00 0 133.3405380 -584678.863  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16400.803  
 7.750600970D+04-1.440779717D+03 1.401744141D+01-6.381631240D-03 5.871674720D-06  
 -2.908872278D-09 5.994050890D-13 -6.579343180D+04-4.494017799D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16400.803  
 -1.378630916D+05-5.579207290D+01 1.004190387D+01-1.682165339D-05 3.724664660D-09  
 -4.275526780D-13 1.982341329D-17 -7.343407470D+04-2.045130429D+01

ALF Gurvich,1996a pt1 p151 pt2 p116.  
 2 tps96 AL 1.00F 1.00 0.00 0.00 0.00 0 45.9799412 -264060.446  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8892.107  
 3.020771686D+04-3.080986949D+02 3.886413140D+00 3.564343690D-03-5.858471280D-06  
 4.388109920D-09-1.256906273D-12 -3.117572862D+04 2.032567172D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8892.107  
 -7.111229050D+05 1.903013316D+03 2.191607179D+00 1.421471467D-03-4.179634770D-07  
 6.153804400D-11-2.945403999D-15 -4.540728960D+04 1.613163743D+01

## Appendix D (continued)

ALF+ Chase,1998 p92.

2 j	6/76 AL	1.00F	1.00E	-1.00	0.00	0.00	0	45.9793926	692233.561
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.643038120D+04	-2.524634478D+02	3.105310486D+00	5.733270430D-03	-8.839786990D-06					
6.343579590D-09	-1.645011685D-12		8.370237450D+04	6.764015580D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.505101126D+06	-2.236668821D+03	3.098216724D+00	3.115413930D-03	-1.168427068D-06					
1.773587168D-10	-9.665841380D-15		9.885083850D+04	5.991894590D+00					

ALFCL Gurvich,1996a pt1 p182 pt2 p144.

2 tpis96 AL	1.00F	1.00CL	1.00	0.00	0.00	0	81.4329412	-436409.913
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.104779480D+04	-5.769646420D+02	6.562642700D+00	4.106285840D-03	-7.213921120D-06				
5.486401450D-09	-1.580656193D-12		-5.114828700D+04	-6.041227053D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.970636350D+04	-6.224485910D+02	7.573475410D+00	-2.236155999D-04	2.382317949D-08				
4.443785760D-12	-5.486977850D-16		-5.100943200D+04	-1.091164505D+01				

ALFCL2 Gurvich,1996a pt1 p183 pt2 p146.

2 tpis96 AL	1.00F	1.00CL	2.00	0.00	0.00	0	116.8859412	-791395.404
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.955607340D+04	-1.188857902D+03	1.156672590D+01	4.574959490D-04	-3.407372830D-06				
3.356822540D-09	-1.085329228D-12		-9.162049260D+04	-3.206065081D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.720360526D+05	-1.193340759D+02	1.008894431D+01	-3.550993810D-05	7.830952610D-09				
-8.961734230D-13	4.145330260D-17		-9.804185470D+04	-2.127046859D+01				

ALF2 Gurvich,1996a pt1 p153 pt2 p117.

2 tpis96 AL	1.00F	2.00	0.00	0.00	0.00	0	64.9783444	-631764.175
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.994951991D+04	-2.194199915D+02	3.416748760D+00	1.272953936D-02	-1.883312206D-05				
1.330702256D-08	-3.680118630D-12		-7.607537650D+04	8.759626916D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.146896245D+05	3.096840150D+01	6.816399620D+00	1.820129379D-04	-7.793677440D-08				
1.472534201D-11	-8.803695300D-16		-7.884002680D+04	-7.915370474D+00				

ALF2- Gurvich,1996a pt1 p154 pt2 p118.

2 tpis96 AL	1.00F	2.00E	1.00	0.00	0.00	0	64.9788930	-853230.685
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.233369037D+05	-1.348195504D+03	8.611178050D+00	2.245141297D-04	-2.424673201D-06				
2.214132430D-09	-6.602713960D-13		-9.708437460D+04	-2.192617549D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.590076965D+05	-2.060486516D+02	7.155289380D+00	-6.260167690D-05	1.391935746D-08				
-1.603901265D-12	7.461508520D-17		-1.040479429D+05	-1.122696648D+01				

ALF2CL Gurvich,1996a pt1 p182 pt2 p145.

2 tpis96 AL	1.00F	2.00CL	1.00	0.00	0.00	0	100.4313444	-999128.145
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.677412090D+04	-8.869829470D+02	8.752746550D+00	8.195791200D-03	-1.380480934D-05				
1.032703706D-08	-2.948968416D-12		-1.177936778D+05	-1.858347360D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.115422988D+05	-1.959188681D+02	1.014576850D+01	-5.813219350D-05	1.281071982D-08				
-1.465366277D-12	6.776002450D-17		-1.227153110D+05	-2.359853398D+01				

ALF3 Gurvich,1996a pt1 p157 pt2 p120.

2 tpis96 AL	1.00F	3.00	0.00	0.00	0.00	0	83.9767476	-1209276.938
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.410263520D+04	-5.667495740D+02	5.833072850D+00	1.603535069D-02	-2.413263602D-05				
1.714106160D-08	-4.747543200D-12		-1.443349991D+05	-5.461613658D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.493972160D+05	-2.911202519D+02	1.021662932D+01	-8.642985970D-05	1.905713108D-08				
-2.181058411D-12	1.009055287D-16		-1.475694276D+05	-2.703983244D+01				

ALF4- Gurvich,1996a pt1 p159 pt2 p121.

2 tpis96 AL	1.00F	4.00E	1.00	0.00	0.00	0	102.9756994	-1951600.806
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.312010037D+05	-3.235376780D+03	2.017865547D+01	-9.108193500D-03	6.679552630D-06				
-2.606075106D-09	4.110060510D-13		-2.211784563D+05	-8.677268282D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.217411610D+05	-2.612097043D+02	1.319792654D+01	-8.010135410D-05	1.786204421D-08				
-2.062751964D-12	9.612581770D-17		-2.381577915D+05	-4.231634322D+01				



## Appendix D (continued)

ALH Gurvich,1996a pt1 p139 pt2 p106.

2 tpis96 AL	1.00H	1.00	0.00	0.00	0.00	0	27.9894780	249250.804
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

-3.759114030D+04 5.089002230D+02 1.128086896D+00 3.988660910D-03-2.150790303D-07

-2.176790819D-09 1.020805902D-12 2.644431827D+04 1.650021856D+01

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

8668.104

6.802018430D+06-2.178416933D+04 3.032713047D+01-1.503343597D-02 4.492142360D-06

-6.178450370D-10 3.115205260D-14 1.658301221D+05-1.876766425D+02

ALHCL Gurvich,1996a pt1 p178 pt2 p138.

2 tpis96 AL	1.00H	1.00CL	1.00	0.00	0.00	0	63.4424780	10521.966
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

10886.572

3.587169760D+04-5.916249990D+02 6.944542380D+00-2.511543148D-03 6.471332550D-06

-5.642277140D-09 1.715950436D-12 2.750930479D+03-9.903745880D+00

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

10886.572

-1.683915330D+05-8.862301790D+02 8.062379400D+00-9.200551470D-04 3.949817220D-07

-6.401086760D-11 3.578354100D-15 3.641504850D+03-1.800686894D+01

ALHCL2 Gurvich,1996a pt1 p179 pt2 p140.

2 tpis96 AL	1.00H	1.00CL	2.00	0.00	0.00	0	98.8954780	-351278.965
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

13676.196

1.184828615D+05-2.054157118D+03 1.574696513D+01-1.476257296D-02 2.065336978D-05

-1.420198850D-08 3.826279860D-12 -3.434277460D+04-5.761184061D+01

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

13676.196

9.608063940D+04-1.485540161D+03 1.103592709D+01-3.956955200D-04 8.465843730D-08

-9.483336520D-12 4.319033530D-16 -3.669216390D+04-3.236862171D+01

ALHF Gurvich,1996a pt1 p164 pt2 p125.

2 tpis96 AL	1.00H	1.00F	1.00	0.00	0.00	0	46.9878812	-182614.484
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

10572.121

-9.289545100D+03 1.335515868D+02 2.772448680D+00 6.751415030D-03-4.133846140D-06

5.865704070D-10 2.276158011D-13 -2.384685845D+04 1.228752581D+01

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

10572.121

7.342169250D+05-3.462164130D+03 1.039714588D+01-1.750737965D-03 4.615687860D-07

-5.390414740D-11 2.340478515D-15 -2.965279722D+03-3.713172313D+01

ALHFCL Gurvich,1996a pt1 p184 pt2 p147.

2 tpis96 AL	1.00H	1.00F	1.00CL	1.00	0.00	0	82.4408812	-555244.524
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

12532.636

1.290373237D+05-2.142099873D+03 1.485434420D+01-1.140326930D-02 1.564521768D-05

-1.067574855D-08 2.857255247D-12 -5.818303070D+04-5.483424986D+01

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

12532.636

4.068987130D+04-1.502129854D+03 1.105214126D+01-4.031587730D-04 8.645252220D-08

-9.700659520D-12 4.423629510D-16 -6.129888110D+04-3.403564016D+01

ALHF2 Gurvich,1996a pt1 p166 pt2 p127.

2 tpis96 AL	1.00H	1.00F	2.00	0.00	0.00	0	65.9862844	-765299.182
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

12299.975

1.050181431D+05-1.398654202D+03 9.166334840D+00 3.867286870D-03-4.830841090D-06

3.099287181D-09-8.440702990D-13 -8.659048800D+04-2.557299683D+01

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

12299.975

-4.419947300D+03-1.612826324D+03 1.113336052D+01-4.351812660D-04 9.344396160D-08

-1.049431425D-11 4.788333980D-16 -8.606916190D+04-3.676383785D+01

ALH2 Gurvich,1996a pt1 p142 pt2 p107.

2 tpis96 AL	1.00H	2.00	0.00	0.00	0.00	0	28.9974180	276774.934
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

10090.834

1.455182996D+04-2.153768996D+02 5.144370230D+00-3.965222030D-03 1.340900203D-05

-1.216744854D-08 3.743107130D-12 3.311037940D+04-3.608799711D+00

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

10090.834

1.432910601D+05-2.365907684D+03 9.085667190D+00-1.308536612D-03 4.777191360D-07

-7.324721890D-11 3.997900940D-15 4.485951850D+04-3.220814285D+01

ALH2CL Gurvich,1996a pt1 p179 pt2 p139.

2 tpis96 AL	1.00H	2.00CL	1.00	0.00	0.00	0	64.4504180	-106345.406
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

11253.251

9.303828980D+04-1.328188016D+03 9.424763590D+00-3.277660590D-03 1.004231609D-05

-8.948123090D-09 2.708031665D-12 -7.647437930D+03-2.682512215D+01

1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								

11253.251

3.166929930D+05-3.094037914D+03 1.215872020D+01-8.248269590D-04 1.765027123D-07

-1.977372723D-11 9.006176280D-16 2.411845642D+03-4.718390855D+01

## Appendix D (continued)

ALH2F                   Gurvich,1996a pt1 p165 pt2 p126.

2 tpis96 AL	1.00H	2.00F	1.00	0.00	0.00	0.00	0	47.9958212	-316655.854
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.906039290D+04	-9.750803930D+02	5.870772320D+00	6.896663690D-03	-4.045817280D-06					
7.219318660D-10	7.329846740D-14		-3.425302600D+04	-9.387539141D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.711514962D+05	-3.169623480D+03	1.221401118D+01	-8.465600260D-04	1.812341995D-07					
-2.030947985D-11	9.251825820D-16		-2.259217746D+04	-4.941337333D+01					

ALH3                   Gurvich,1996a pt1 p145 pt2 p109.

2 tpis96 AL	1.00H	3.00	0.00	0.00	0.00	0	30.0053580	128896.080
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.481207909D+04	-2.836495340D+01	2.507597126D+00	7.315920510D-03	2.331766687D-06				
-6.389209890D-09	2.456885069D-12		1.463189428D+04	8.313187700D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.885458550D+05	-4.595785660D+03	1.320893344D+01	-1.226849004D-03	2.626580824D-07				
-2.943725869D-11	1.341177648D-15		3.991716950D+04	-6.181829295D+01				

ALI                   Gurvich,1996a pt1 p191 pt2 p153.

2 tpis96 AL	1.00I	1.00	0.00	0.00	0.00	0	153.8860080	67395.017
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.870854131D+03	-1.543184003D+02	5.074391880D+00	-1.120584830D-03	1.386302156D-06				
-8.540782280D-10	2.180358492D-13		7.517443690D+03	6.688267622D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.752817920D+05	-1.198028588D+03	5.433685360D+00	-1.004479306D-04	-1.005928846D-07				
4.568173190D-11	-3.960201360D-15		1.464627816D+04	-3.141199746D+00				

ALI2                   Gurvich,1996a pt1 p193 pt2 p154.

2 tpis96 AL	1.00I	2.00	0.00	0.00	0.00	0	280.7904780	-33812.954
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.423413595D+04	-4.646575690D+02	8.722674910D+00	-3.560519290D-03	4.188682290D-06				
-2.616026962D-09	6.720195510D-13		-3.846133330D+03	-1.073076578D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.35599020D+05	4.743347940D+02	7.106501390D+00	-5.529965340D-04	3.161480314D-07				
-5.515489160D-11	3.174155820D-15		-9.785488850D+03	-5.602275944D-01				

ALI3                   Gurvich,1996a pt1 p195 pt2 p156.

2 tpis96 AL	1.00I	3.00	0.00	0.00	0.00	0	407.6949480	-191330.433
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.706032439D+04	-7.559936810D+02	1.271396349D+01	-5.466884090D-03	6.297618920D-06				
-3.864209610D-09	9.774132440D-13		-2.220966921D+04	-2.847883861D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.357427470D+04	-1.578772280D+01	1.001249733D+01	-5.228673120D-06	1.196173520D-09				
-1.409194490D-13	6.671276390D-18		-2.611455525D+04	-1.247999813D+01				

ALN                   Gurvich,1996a pt1 p204 pt2 p164.

2 tpis96 AL	1.00N	1.00	0.00	0.00	0.00	0	40.9882380	438829.011
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.716645079D+04	-2.543491110D+02	3.538987720D+00	5.296256160D-03	-9.845700610D-06				
8.452209040D-09	-2.592304568D-12		5.309994910D+04	5.399435220D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.821214220D+06	-1.067776595D+04	1.449174222D+01	-3.727227130D-03	7.922770960D-07				
-8.086892210D-11	2.893539736D-15		1.205236340D+05	-7.288585119D+01				

ALO                   Gurvich,1996a pt1 p122 pt2 p96.

3 tpis96 AL	1.000	1.00	0.00	0.00	0.00	0	42.9809380	67319.006
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.683391100D+03	2.957969549D+02	4.808108440D-01	1.169224855D-02	-1.595428871D-05				
1.060766814D-08	-2.647888708D-12		5.843672170D+03	2.160997839D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.565721161D+04	3.855741010D+03	-5.926079780D+00	9.050960420D-03	-2.930661549D-06				
4.238529070D-10	2.280655341D-14		-1.331694655D+04	6.830663436D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.165661210D+07	-3.768608760D+04	1.547867956D+01	-9.568730340D-04	2.493109541D-08				
6.688940290D-14	-8.998673700D-18		2.957786517D+05	-9.427715804D+01				

ALO+                   Chase,1998 p133.

2 j12/79 AL	1.000	1.00E	-1.00	0.00	0.00	0	42.9803894	992993.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.829178513D+04	-4.179087100D+02	5.313299870D+00	-1.410883046D-03	2.526524021D-06				
-2.005474816D-09	5.762553550D-13		1.203648109D+05	-3.410565930D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.710846446D+04	-6.998653420D+02	5.787815840D+00	-6.871895460D-04	2.075047303D-07				
-2.655281004D-11	1.283129660D-15		1.218682226D+05	-7.051035880D+00				

## Appendix D (continued)

ALO- Gurvich,1996a pt1 p125 pt2 p98.  
 2 g11/97 AL 1.000 1.00E 1.00 0.00 0.00 0 42.9814866 -272921.782  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8744.718  
 2.078075267D+04 2.859351226D+00 1.901912370D+00 7.301045660D-03-9.139769870D-06  
 5.652983190D-09-1.396787103D-12 -3.359267730D+04 1.296339858D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8744.718  
 -6.971948290D+04-2.320553036D+02 4.672784330D+00-4.266447040D-05 1.632506336D-08  
 -1.727134051D-12 8.136840640D-17 -3.307718930D+04-2.155922595D+00

ALOCL Gurvich,1996a pt1 p176 pt2 p136.  
 2 tpis96 AL 1.000 1.00CL 1.00 0.00 0.00 0 78.4339380 -301564.570  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11906.037  
 -5.144627790D+03-5.886297070D+01 4.452316930D+00 9.288235090D-03-1.246894823D-05  
 8.178073540D-09-2.130739934D-12 -3.759683650D+04 2.476862818D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11906.037  
 -1.258027706D+05-2.420565961D+02 7.681130020D+00-7.268741700D-05 1.611337534D-08  
 1.852889749D-12 8.607278220D-17 -3.754326050D+04-1.475818320D+01

ALOCL2 Gurvich,1996a pt1 p178 pt2 p137.  
 2 tpis96 AL 1.000 1.00CL 2.00 0.00 0.00 0 113.8869380 -402308.669  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15752.494  
 6.902637130D+04-1.189297500D+03 1.161842739D+01 2.818279805D-04-3.145010615D-06  
 3.168380650D-09-1.032375462D-12 -4.483323070D+04-3.165475132D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15752.494  
 -1.707713922D+05-1.180013804D+02 1.008798517D+01-3.513858040D-05 7.751187030D-09  
 -8.872470600D-13 4.104815440D-17 -5.124944140D+04-2.059252960D+01

ALOF Gurvich,1996a pt1 p163 pt2 p123.  
 2 tpis96 AL 1.000 1.00F 1.00 0.00 0.00 0 61.9793412 -572289.603  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11003.003  
 7.030578360D+03-1.154575430D+02 3.378823590D+00 1.283929158D-02-1.749748388D-05  
 1.162605473D-08-3.064218613D-12 -6.959381700D+04 5.994804586D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11003.003  
 -1.641020297D+05-3.277770290D+02 7.744519740D+00-9.788649440D-05 2.165743208D-08  
 -2.486541919D-12 1.153633944D-16 -6.974085090D+04-1.717253748D+01

ALOF2 Gurvich,1996a pt1 p164 pt2 p124.  
 2 tpis96 AL 1.000 1.00F 2.00 0.00 0.00 0 80.9777444 -773649.771  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14055.387  
 4.756085290D+04-6.124318360D+02 6.050223660D+00 1.559291479D-02-2.366136797D-05  
 1.688366194D-08-4.690583100D-12 -9.171827490D+04-4.956258224D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14055.387  
 -2.389881459D+05-2.837821503D+02 1.021108125D+01-8.418303430D-05 1.855520828D-08  
 -2.122974022D-12 9.819319100D-17 -9.521804190D+04-2.522534812D+01

ALOF2- Chase,1998 p98 6/76.  
 2 g 2/01 AL 1.000 1.00F 2.00E 1.00 0.00 0 80.9782930 -972289.619  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14076.981  
 1.540605112D+05-1.928054597D+03 1.255806423D+01-4.904035370D-04-2.341783347D-06  
 2.415138600D-09-7.471809250D-13 -1.091430174D+05-4.265821750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14076.981  
 -2.389881459D+05-2.880143725D+02 1.021700240D+01-8.747062000D-05 1.944846334D-08  
 -2.241045051D-12 1.042591053D-16 -1.190576566D+05-2.600779629D+01

ALOH Gurvich,1996a pt1 p145 pt2 p110.  
 2 tpis96 AL 1.000 1.00H 1.00 0.00 0.00 0 43.9888780 -192762.171  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10351.931  
 5.876493180D+04-9.449422690D+02 7.820599180D+00 5.858888470D-04-4.083666810D-06  
 4.587229340D-09-1.563936726D-12 -1.993283011D+04-2.065043885D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10351.931  
 7.882068110D+05-2.263671626D+03 7.823954880D+00 1.821171456D-04-8.263729320D-08  
 1.265414876D-11-6.875972530D-16 -1.039808093D+04-2.209032458D+01

ALOHCL Gurvich,1996a pt1 p180 pt2 p141.  
 2 tpis96 AL 1.000 1.00H 1.00CL 1.00 0.00 0 79.4418780 -373785.740  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13918.918  
 1.636360341D+04-1.915959416D+02 4.711170470D+00 1.388068475D-02-1.999018454D-05  
 1.439647350D-08-4.033330450D-12 -4.568083720D+04 4.644207506D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13918.918  
 7.967115510D+05-2.843470502D+03 1.095559970D+01-1.099328162D-04-1.344506283D-08  
 4.415893770D-12-2.973546112D-16 -2.969861461D+04-3.296113996D+01

## Appendix D (continued)

ALOHCL2                    Gurvich,1996a pt1 p181 pt2 p143.  
 2 tps96 AL 1.000 1.00H 1.00CL 2.00 0.00 0 114.8948780 -725145.408  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17149.806  
 3.971929860D+04-7.751554960D+02 9.494051530D+00 1.074401359D-02-1.676464791D-05  
 1.259706368D-08-3.613177980D-12 -8.584796930D+04-1.993481642D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17149.806  
 7.385929760D+05-2.863204228D+03 1.397062327D+01-1.160311527D-04-1.208248796D-08  
 4.258327630D-12-2.900049181D-16 -7.293048000D+04-4.681834857D+01

ALOHF                    Gurvich,1996a pt1 p166 pt2 p128.  
 2 tps96 AL 1.000 1.00H 1.00F 1.00 0.00 0 62.9872812 -574211.575  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13315.081  
 -1.556003336D+03 2.886581999D+02 7.703793290D-01 2.450406329D-02-3.417811010D-05  
 2.388932902D-08-6.570480510D-12 -7.177222560D+04 2.453071801D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13315.081  
 7.557113130D+05-2.936702803D+03 1.102455104D+01-1.373078030D-04-7.432816160D-09  
 3.729981220D-12-2.657027781D-16 -5.340130900D+04-3.527397302D+01

ALOHF2                    Gurvich,1996a pt1 p168 pt2 p130.  
 2 tps96 AL 1.000 1.00H 1.00F 2.00 0.00 0 81.9856844 -1141510.711  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15428.498  
 1.738263538D+04-1.307687299D+02 3.312381920D+00 2.784734099D-02-3.982363210D-05  
 2.809344456D-08-7.764574200D-12 -1.384133568D+05 1.004739945D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15428.498  
 6.530119920D+05-3.034017232D+03 1.409719788D+01-1.663681799D-04-1.011564183D-09  
 2.993805003D-12-2.315956955D-16 -1.223052213D+05-5.151210690D+01

ALO2                    Gurvich,1996a pt1 p126 pt2 p99.  
 2 tps96 AL 1.000 2.00 0.00 0.00 0.00 0 58.9803380 -38657.871  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13361.629  
 4.338480450D+04-4.735292260D+02 6.001717670D+00 7.094420880D-03-1.129107996D-05  
 8.252691680D-09-2.327652976D-12 -3.826145800D+03-4.830022480D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13361.629  
 1.187216642D+05-8.335625400D+02 8.309301190D+00-3.538667220D-04 5.967069460D-08  
 4.014897700D-14-3.515702520D-16 -2.033107586D+03-1.715063884D+01

ALO2-                    Gurvich,1996a pt1 p128 pt2 p100.  
 2 tps96 AL 1.000 2.00E 1.00 0.00 0.00 0 58.9808866 -452572.223  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10644.677  
 1.178678641D+05-1.507186304D+03 9.524749750D+00-5.207989020D-04-1.586902345D-06  
 1.700455028D-09-5.301419770D-13 -4.825469270D+04-3.081215859D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10644.677  
 -1.872410758D+05-2.338853263D+02 7.676070020D+00-7.093570300D-05 1.576717569D-08  
 -1.816494162D-12 8.449707960D-17 -5.594640560D+04-1.773751567D+01

AL(OH)2                    Gurvich,1996a pt1 p149 pt2 p113.  
 2 tps96 AL 1.000 2.00H 2.00 0.00 0.00 0 60.9962180 -507660.670  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14027.535  
 4.397316910D+03 1.327680339D+02 1.093947024D+00 3.054059173D-02-4.375943350D-05  
 3.174617430D-08-9.004259400D-12 -6.315437390D+04 2.101977655D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14027.535  
 1.669643735D+06-5.924738280D+03 1.549480264D+01-5.383488080D-04 5.413044530D-08  
 -1.196022328D-12-1.082001733D-16 -2.697525061D+04-6.617911543D+01

AL(OH)2CL                    Gurvich,1996a pt1 p181 pt2 p142.  
 2 tps96 AL 1.000 2.00H 2.00CL 1.00 0.00 0 96.4492180 -859056.724  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17222.037  
 2.477879709D+04-4.454577210D+02 5.928470200D+00 2.730162734D-02-4.041405370D-05  
 2.974210410D-08-8.477150600D-12 -1.033778030D+05-3.679940779D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17222.037  
 1.603911487D+06-5.767232240D+03 1.817772266D+01-3.691816150D-04 1.137918702D-08  
 4.083079400D-12-3.641323430D-16 -7.118699850D+04-7.757541774D+01

AL(OH)2F                    Gurvich,1996a pt1 p167 pt2 p129.  
 2 tps96 AL 1.000 2.00H 2.00F 1.00 0.00 0 79.9946212 -1069628.708  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16472.051  
 2.132812662D+04-1.932900224D+02 3.069174664D+00 3.555017330D-02-5.181158330D-05  
 3.753520280D-08-1.059220701D-11 -1.295797992D+05 1.001897011D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16472.051  
 1.559238236D+06-5.841273030D+03 1.823229919D+01-3.907805420D-04 1.610928938D-08  
 3.544784060D-12-3.393453880D-16 -9.623100890D+04-7.971351802D+01

## Appendix D (continued)

AL(OH)3                      Gurvich,1996a pt1 p150 pt2 p115.  
 2 tpis96 AL 1.000 3.00H 3.00 0.00 0.00 0 78.0035580 -1012667.542  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17594.767  
 -1.402475452D+04 3.696073460D+02-2.979600650D-01 4.929859350D-02-6.981572280D-05  
 5.014801700D-08-1.412480165D-11 -1.255260760D+05 2.711490074D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17594.767  
 2.477063616D+06-8.968617250D+03 2.280320998D+01-8.320292250D-04 8.663494430D-08  
 -2.420287082D-12-1.331746442D-16 -7.015278640D+04-1.121899198D+02

ALS                              Gurvich,1996a pt1 p197 pt2 p158.  
 2 tpis96 AL 1.00S 1.00 0.00 0.00 0.00 0 59.0465380 232682.009  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9088.109  
 2.611742801D+04-3.470673890D+02 4.436204590D+00 3.340168210D-03-8.410199670D-06  
 8.508185110D-09-2.780868507D-12 2.863779062D+04 7.522705491D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9088.109  
 8.909844290D+06-2.507677454D+04 2.893456134D+01-9.839766820D-03 2.045319809D-06  
 -2.087970890D-10 8.152792520D-15 1.885761615D+05-1.786036457D+02

ALS2                             Gurvich,1996a pt1 p198 pt2 p159.  
 2 tpis96 AL 1.00S 2.00 0.00 0.00 0.00 0 91.1115380 248535.279  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14428.779  
 4.252335410D+04-7.764603300D+02 9.801068960D+00-3.910680090D-03 3.875695970D-06  
 -2.082025593D-09 4.682935890D-13 3.167961540D+04-2.178097896D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14428.779  
 -6.852563540D+04-2.671667739D+01 7.520193860D+00-8.148565100D-06 1.811865152D-09  
 -2.086958125D-13 9.703246380D-18 2.758362737D+04-7.873490263D+00

AL2                               Gurvich,1996a pt1 p118 pt2 p95.  
 2 tpis96 AL 2.00 0.00 0.00 0.00 0.00 0 53.9630760 501301.722  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10139.122  
 -5.281509650D+03-1.727374523D+01 4.604077010D+00-2.616467770D-04 6.302319970D-07  
 -3.290938590D-10 8.888365140D-14 5.900706390D+04 3.060188921D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10139.122  
 -2.320724102D+06 9.218707890D+03-9.446951870D+00 9.999920010D-03-3.154798085D-06  
 4.361544810D-10-2.241157240D-14 2.904589544D+03 9.960320745D+01

AL2Br6                         Gurvich,1996a pt1 p190 pt2 p152.  
 2 tpis96 AL 2.00BR 6.00 0.00 0.00 0.00 0 533.3870760 -942422.811  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38217.189  
 6.483319700D+04-1.947687811D+03 2.886989822D+01-1.365825785D-02 1.557883731D-05  
 -9.486942000D-09 2.385519396D-12 -1.101526833D+05-1.025934782D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38217.189  
 -1.731829490D+05-4.342299780D+01 2.203414210D+01-1.421187503D-05 3.238631340D-09  
 -3.803879760D-13 1.796525455D-17 -1.202338355D+05-6.201054950D+01

AL2C2                            Gurvich,1996a pt1 p206 pt2 p167.  
 2 tpis96 AL 2.00C 2.00 0.00 0.00 0.00 0 77.9844760 544978.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16165.001  
 1.110987147D+04-3.502434230D+02 8.598856000D+00 1.832528671D-03 1.035743392D-06  
 -2.091649890D-09 7.716068700D-13 6.492764190D+04-1.645080239D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16165.001  
 1.597651967D+05-1.644007203D+03 1.164643675D+01-4.379215430D-04 9.369640110D-08  
 -1.049615854D-11 4.780468930D-16 7.204889810D+04-3.648164252D+01

AL2CL6                         Gurvich,1996a pt1 p175 pt2 p135.  
 2 tpis96 AL 2.00CL 6.00 0.00 0.00 0.00 0 266.6810760 -1296876.242  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 34147.090  
 1.340935279D+05-3.001037953D+03 3.143000879D+01-1.700408496D-02 1.786540089D-05  
 -1.015419943D-08 2.409630451D-12 -1.471830046D+05-1.274445324D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 34147.090  
 -2.752975554D+05-9.248235970D+01 2.207058224D+01-2.870537915D-05 6.423325690D-09  
 -7.436585200D-13 3.472064670D-17 -1.629157014D+05-7.091602129D+01

AL2F6                            Gurvich,1996a pt1 p160 pt2 p122.  
 2 tpis96 AL 2.00F 6.00 0.00 0.00 0.00 0 167.9534952 -2632491.231  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26064.089  
 1.915061289D+05-3.168240250D+03 2.245374802D+01 1.271532036D-02-2.488697302D-05  
 1.955252096D-08-5.712084890D-12 -3.049962550D+05-9.396473101D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26064.089  
 -5.852982610D+05-5.450571990D+02 2.240686320D+01-1.627323704D-04 3.595225040D-08  
 -4.121201440D-12 1.909095384D-16 -3.219683910D+05-8.589867941D+01

## Appendix D (continued)

AL2I6 Gurvich,1996a pt1 p196 pt2 p157.  
 2 tps96 AL 2.00I 6.00 0.00 0.00 0.00 0.00 0 815.3898960 -487747.035  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 40920.966  
 2.587571514D+04-1.280719742D+03 2.677715820D+01-9.913018470D-03 1.168760413D-05  
 -7.303918530D-09 1.874532749D-12 -5.891105550D+04-8.330209321D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 40920.966  
 -1.210112399D+05-2.467542774D+01 2.201992650D+01-8.462022590D-06 1.957831901D-09  
 -2.326573151D-13 1.108910373D-17 -6.548523750D+04-5.528536481D+01

AL2O Gurvich,1996a pt1 p129 pt2 p101.  
 2 tps96 AL 2.000 1.00 0.00 0.00 0.00 0 69.9624760 -148611.286  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12776.514  
 7.776530700D+03-1.294235361D+02 4.912509520D+00 8.604223450D-03-1.217703648D-05  
 8.314634870D-09-2.237722201D-12 -1.886512879D+04-2.806368311D-02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12776.514  
 -1.171074351D+05-1.783009166D+02 7.633215360D+00-5.335931770D-05 1.180702791D-08  
 -1.355444579D-12 6.287323890D-17 -1.947580149D+04-1.415764167D+01

AL2O+ Chase,1998 p151 12/79.  
 2 g 1/01 AL 2.000 1.00E -1.00 0.00 0.00 0 69.9619274 648970.248  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12981.148  
 6.828925720D+04-9.098504170D+02 8.896563010D+00-7.772554380D-04-4.034655620D-07  
 6.977315050D-10-2.417262484D-13 8.085007550D+04-2.176216731D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12981.148  
 -1.102225105D+05-1.214571732D+02 7.591595950D+00-3.694539160D-05 8.218520320D-09  
 -9.473649720D-13 4.408621350D-17 7.614943580D+04-1.282233856D+01

AL2O2 Gurvich,1996a pt1 p131 pt2 p102.  
 2 tps96 AL 2.000 2.00 0.00 0.00 0.00 0 85.9618760 -403095.587  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15842.613  
 -1.940560042D+04 2.508489836D+02 3.621403790D+00 1.951385302D-02-2.560329071D-05  
 1.662721576D-08-4.312396200D-12 -5.172697280D+04 9.923995945D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15842.613  
 -1.940611656D+05-4.609752430D+02 1.084375637D+01-1.376042893D-04 3.044733119D-08  
 -3.496193920D-12 1.622305079D-16 -4.963055780D+04-2.946538090D+01

AL2O2+ Chase,1998 p153 12/79.  
 2 g 2/01 AL 2.000 2.00E -1.00 0.00 0.00 0 85.9613274 557438.835  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14975.135  
 8.292034990D+04-1.757427015D+03 1.525328567D+01-8.983131330D-03 8.953954500D-06  
 -4.840586200D-09 1.096696856D-12 7.311677140D+04-5.517092550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14975.135  
 -1.652005184D+05-6.021606970D+01 1.004626917D+01-1.892194088D-05 4.253301200D-09  
 -4.942390420D-13 2.314507373D-17 6.386219000D+04-2.345753361D+01

AL2O3 Gurvich,1996a pt1 p137 pt2 p105.  
 2 tps96 AL 2.000 3.00 0.00 0.00 0.00 0 101.9612760 -546890.530  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19598.070  
 -7.443374320D+03 8.829004210D+01 5.264662640D+00 2.507678848D-02-3.434541650D-05  
 2.302516980D-08-6.122529280D-12 -6.872685950D+04 2.202324298D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19598.070  
 -2.777784969D+05-4.917465930D+02 1.386703888D+01-1.469381940D-04 3.250406490D-08  
 -3.730867350D-12 1.730444284D-16 -6.790757850D+04-4.375559873D+01

AL2S Gurvich,1996a pt1 p199 pt2 p160.  
 2 tps96 AL 2.00S 1.00 0.00 0.00 0.00 0 86.0280760 220679.131  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14003.931  
 4.094624370D+04-7.797172470D+02 9.814423100D+00-3.940339820D-03 3.912465430D-06  
 -2.105891677D-09 4.746001080D-13 2.833963305D+04-2.465067552D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14003.931  
 -7.043437370D+04-2.676376869D+01 7.520233820D+00-8.166123060D-06 1.816026040D-09  
 -2.091989298D-13 9.727537700D-18 2.422718377D+04-1.066580982D+01

AL2S2 Gurvich,1996a pt1 p200 pt2 p161.  
 2 tps96 AL 2.00S 2.00 0.00 0.00 0.00 0 118.0930760 135287.321  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18099.521  
 6.614587320D+04-1.111319537D+03 1.257007304D+01-1.456053256D-03-5.851627110D-07  
 1.390055053D-09-5.496468200D-13 1.914456895D+04-3.600277092D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18099.521  
 -1.377806456D+05-7.705032500D+01 1.055723566D+01-2.277554487D-05 5.007682850D-09  
 -5.715862120D-13 2.637999240D-17 1.313336091D+04-2.256851594D+01

## Appendix D (continued)

Ar                      Ref-Elm. Moore,1971. Gordon,1999.

3 g 3/98 AR	1.00	0.00	0.00	0.00	0.00	0.00	0	39.9480000	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+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
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.010538475D+01	-5.992661070D-02	2.500069401D+00	-3.992141160D-08	1.205272140D-11					
-1.819015576D-15	1.078576636D-19								-7.449939610D+02
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.951265080D+08	6.458887260D+05	-1.675894697D+02	2.319933363D-02	-1.721080911D-06					
6.531938460D-11	-9.740147729D-16								-5.078300340D+06
									1.465298484D+03

Ar+                      Moore,1971. IP:Moore,1970a. Gordon,1999.

3 g 1/99 AR	1.00E	-1.00	0.00	0.00	0.00	0.00	0	39.9474514	1526778.407
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.731209170D+04	7.930791470D+02	-1.717121217D+00	1.044184018D-02	-1.180207501D-05					
6.528134780D-09	-1.447558130D-12								1.790572230D+05
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.835965400D+05	8.162019700D+02	2.301342628D+00	-4.952983770D-06	1.205108477D-08					
-2.185050286D-12	1.265493898D-16								1.771811455D+05
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.006884827D+07	-6.624361280D+03	4.446908200D+00	-3.017567664D-04	2.612882069D-08					
-1.201637769D-12	2.299206903D-17								2.349504137D+05
									-1.032262257D+01

B                      Martin,1998. Odintzova,1979. Gordon,1999.

3 g 9/98 B	1.00	0.00	0.00	0.00	0.00	0.00	0	10.8110000	575598.760
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.182394638D+02	-7.009916910D-02	2.500236159D+00	-4.584213700D-07	5.123185830D-10					
-3.057217674D-13	7.533815325D-17								6.848359080D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.072659610D+05	3.225307160D+02	2.126407232D+00	2.106579339D-04	-5.937129160D-08					
7.377427990D-12	-2.282443381D-16								6.643413100D+04
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.150001310D+08	2.329576796D+05	-4.720913710D+01	4.877655960D-03	-2.069413791D-07					
3.233519090D-12	-1.824076527D-18								-1.802904743D+06
									4.439617640D+02

B+                      Moore,1971. IP:Moore,1970a. Gordon,1999.

3 g 9/98 B	1.00E	-1.00	0.00	0.00	0.00	0.00	0	10.8104514	1382315.528
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.849791190D-02	-8.947480950D-04	2.500004085D+00	-9.577271230D-09	1.218136411D-11					
-7.986752520D-15	2.113769829D-18								1.655080260D+05
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.911548030D+03	4.587790090D+00	2.531500086D+00	-4.903949100D-05	2.853326582D-08					
-7.382175910D-12	7.120721560D-16								1.654526303D+05
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.977322890D+08	4.734044940D+05	-1.055286044D+02	1.170310076D-02	-6.075531110D-07					
1.484174716D-11	-1.328323987D-16								-3.609116960D+06
									9.497399750D+02

B-                      Hotop,1985. Gordon,1999.

3 g 9/98 B	1.00E	1.00	0.00	0.00	0.00	0.00	0	10.8115486	542631.498
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.201568105D+01	-4.740468880D-03	2.500014238D+00	-2.497056599D-08	2.556360708D-11					
-1.415274780D-14	3.271770710D-18								6.451791880D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.118018248D+01	2.070697496D-04	2.499999729D+00	1.456693631D-10	-3.888571760D-14					
5.090598630D-12	-2.601566168D-22								6.451789140D+04
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.311386485D+02	9.028908800D-02	2.499978572D+00	2.606391052D-09	-1.716068068D-13					
5.810865540D-18	-7.925029090D-23								6.451717400D+04
									4.616640300D+00

BBr                      Gurvich,1996a pt1 p91 pt2 p70.

2 g 9/98 B	1.00BR	1.00	0.00	0.00	0.00	0.00	0	90.7150000	240952.358
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.796093500D+04	-4.976096020D+02	5.267008200D+00	-3.742840190D-05	-1.131544370D-06					
1.261945702D-09	-4.288811880D-13								3.038125367D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.536858027D+05	-6.405909500D+02	4.666823470D+00	4.175486390D-04	-2.963714868D-07					
7.519119540D-11	-4.835368320D-15								3.189084340D+04
									-8.255870910D-01

BBr2                      Gurvich,1996a pt1 p92 pt2 p71.

2 g 9/98 B	1.00BR	2.00	0.00	0.00	0.00	0.00	0	170.6190000	97828.617
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.516550710D+04	-9.029590760D+02	8.063817800D+00	1.129849010D-03	-4.195482390D-06					
3.965658770D-09	-1.283029835D-12								1.470466408D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.191633370D+05	4.157688470D+02	7.148169830D+00	-5.689590750D-04	3.195441770D-07					
-5.553176990D-11	3.191136760D-15								6.118982050D+03
									-5.502759620D+00

## Appendix D (continued)

BBr3                      Gurvich,1996a pt1 p93 pt2 p72.  
 2 tps96 B    1.00BR   3.00   0.00   0.00   0.00 0   250.5230000   -205300.000  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       15702.797  
     3.968073690D+04-6.331087160D+02 8.054551570D+00 9.777571300D-03-1.614866025D-05  
     1.216119883D-08-3.516539610D-12                      -2.366723308D+04-1.106099390D+01  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       15702.797  
 -1.901046795D+05-1.503627687D+02 1.010999896D+01-4.323095110D-05 9.409696190D-09  
 -1.065218470D-12 4.883048770D-17                      -2.742553062D+04-1.997496003D+01

BC                      Gurvich,1996a pt1 p108 pt2 p86.  
 2 g 9/98 B    1.00C    1.00   0.00   0.00   0.00 0   22.8217000       838161.905  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       8735.105  
 -3.915758000D+04 7.284538060D+02-1.552743361D+00 1.552898673D-02-1.976857863D-05  
     1.272066405D-08-3.229982780D-12                      9.644913680D+04 3.248204466D+01  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       8735.105  
 -2.346280674D+06 6.450751300D+03-2.619532384D+00 3.339160500D-03-4.508022140D-07  
     1.351919576D-11 8.265104270D-16                      5.786685070D+04 5.037884876D+01

BC2                      Gurvich,1996a pt1 p109 pt2 p87.  
 2 g 9/98 B    1.00C    2.00   0.00   0.00   0.00 0   34.8324000       801258.725  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       11687.825  
 -2.987422175D+04 3.643126580D+02 2.963469415D+00 6.561750150D-03-3.539767240D-06  
     1.927356029D-10 3.118724866D-13                      9.304835730D+04 1.083424193D+01  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       11687.825  
     1.525485889D+06-5.987862380D+03 1.408384855D+01-3.747499800D-03 1.081927223D-06  
 -1.378744645D-10 6.473822000D-15                      1.311204013D+05-6.337215498D+01

BCL                      Gurvich,1996a pt1 p73 pt2 p51.  
 2 g 9/98 B    1.00CL   1.00   0.00   0.00   0.00 0   46.2640000       183173.437  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       8861.337  
     2.202458989D+04-1.700511155D+02 3.066075869D+00 5.595070180D-03-8.460870410D-06  
     6.084733410D-09-1.702889433D-12                      2.197402537D+04 6.388978917D+00  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       8861.337  
 -7.421262540D+04 2.638090127D+02 3.600227650D+00 1.018866266D-03-4.666184120D-07  
     9.849002030D-11-6.468818170D-15                      1.912726480D+04 5.235317877D+00

BCL+                      Chase,1998 p198.  
 2 j 6/68 B    1.00CL   1.00E   -1.00   0.00   0.00 0   46.2634514       1234280.000  
     298.150   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       8860.318  
     6.514405420D+04-6.845541010D+02 5.527276820D+00-4.458357450D-04-4.557728840D-07  
     6.370858160D-10-2.134366120D-13                      1.509424507D+05-6.918246393D+00  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       8860.318  
 -2.169423542D+05 3.589975160D+02 4.035208370D+00 3.274452430D-04-8.634578450D-08  
     1.207061044D-11-5.262253270D-16                      1.445477224D+05 3.488222017D+00

BCLOH                      Gurvich,1996a pt1 p83 pt2 p61.  
 2 g 9/98 B    1.00CL   1.00O   1.00H   1.00   0.00 0   63.2713400       -234005.381  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       12431.519  
 -2.898427288D+04 6.894046580D+02-2.288138069D+00 3.349428620D-02-4.725225980D-05  
     3.326981310D-08-9.224238860D-12                      -3.261981100D+04 3.976886651D+01  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       12431.519  
     7.027738440D+05-2.857391274D+03 1.091175840D+01-8.107709340D-05-2.124440337D-08  
     5.409912440D-12-3.464153840D-16                      -1.307221888D+04-3.585168799D+01

BCL(OH)2                      Gurvich,1996a pt1 p85 pt2 p62.  
 2 tps96 B    1.00CL   1.00O   2.00H   2.00   0.00 0   80.2786800       -805387.658  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       13565.103  
     8.072623010D+04-8.594619820D+02 2.705039614D+00 3.878799620D-02-5.721734350D-05  
     4.145850330D-08-1.168536754D-11                      -9.379910740D+04 7.134982695D+00  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       13565.103  
     1.423878191D+06-5.849704070D+03 1.792165219D+01-2.009909087D-04-3.393435780D-08  
     9.838560760D-12-6.472678820D-16                      -6.474261760D+04-8.100399519D+01

BCL2                      Gurvich,1996a pt1 p74 pt2 p52.  
 2 tps96 B    1.00CL   2.00   0.00   0.00   0.00 0   81.7170000       -60881.490  
     200.000   1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       11513.621  
     3.598879420D+04-3.602826500D+02 4.157685450D+00 1.152877450D-02-1.816567395D-05  
     1.341714418D-08-3.840822860D-12                      -6.765107050D+03 5.182311874D+00  
     1000.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0       11513.621  
     3.501403130D+05-1.662203590D+03 8.839534720D+00-9.772544110D-04 2.467356248D-07  
 -2.501151018D-11 8.722954560D-16                      5.682909440D+02-2.148348344D+01



## Appendix D (continued)

BCL2+ Chase,1998 p203 12/79.

2 g 1/01 B	1.00CL	2.00E	-1.00	0.00	0.00	0	81.7164514	672315.402
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12848.802
8.065956240D+04	-1.149602601D+03	1.016765297D+01	-3.586494910D-03	2.837145924D-06				
-1.225075731D-09	2.224794198D-13		8.478617410D+04	-2.937256994D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12848.802
3.029293331D+05	-1.305533159D+03	8.920390060D+00	-7.289919640D-04	1.727833266D-07				
-1.523567337D-11	4.226911440D-16		8.653415770D+04	-2.267466616D+01				

BCL2OH Gurvich,1996a pt1 p86 pt2 p63.

2 tpis96 B	1.00CL	2.000	1.00H	1.00	0.00	0	98.7243400	-604917.444
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								14051.769
2.099755170D+04	-2.470699169D+02	2.578761742D+00	3.120362393D-02	-4.545314050D-05				
3.242011770D-08	-9.039822660D-12		-7.309028620D+04	1.273658611D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								14051.769
5.878113790D+05	-2.982969317D+03	1.400662004D+01	-1.194189832D-04	-1.269775742D-08				
4.422892190D-12	-3.004089365D-16		-5.824168070D+04	-5.150858228D+01				

BCL3 Gurvich,1996a pt1 p76 pt2 p53.

2 tpis96 B	1.00CL	3.00	0.00	0.00	0.00	0	117.1700000	-404500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								13970.666
2.392970339D+04	-4.140378860D+02	5.488035260D+00	1.648395682D-02	-2.456196216D-05				
1.743876340D-08	-4.845222140D-12		-4.839469840D+04	-1.675355198D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								13970.666
-2.417408819D+05	-2.921539509D+02	1.021668480D+01	-8.623637100D-05	1.897792088D-08				
-2.168726841D-12	1.002154013D-16		-5.074834440D+04	-2.546862377D+01				

BF Gurvich,1996a pt1 p56 pt2 p36.

2 g10/97 B	1.00F	1.00	0.00	0.00	0.00	0	29.8094032	-106931.884
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8694.670
-5.238954730D+04	8.118476640D+02	-1.141614903D+00	1.161249417D-02	-1.175212617D-05				
6.019232780D-09	-1.238293129D-12		-1.774541998D+04	3.005086287D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8694.670
-3.746389780D+05	5.604493910D+02	3.609186110D+00	6.187216930D-04	-1.778938770D-07				
2.426601527D-11	-9.394651580D-16		-1.819179292D+04	3.716609290D+00				

BFCL Gurvich,1996a pt1 p86 pt2 p64.

2 tpis96 B	1.00F	1.00CL	1.00	0.00	0.00	0	65.2624032	-279184.068
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11033.040
-2.363512735D+04	4.383168980D+02	3.918095720D-01	1.719990692D-02	-2.139592424D-05				
1.337389186D-08	-3.371164690D-12		-3.687166590D+04	2.668102752D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11033.040
-1.086309561D+05	-5.233438480D+02	7.297504740D+00	-3.054410701D-05	-3.154598306D-08				
1.052290533D-11	-7.615432260D-16		-3.305891210D+04	-1.186586595D+01				

BFCL2 Gurvich,1996a pt1 p88 pt2 p66.

2 tpis96 B	1.00F	1.00CL	2.00	0.00	0.00	0	100.7154032	-643000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								13230.913
4.402551240D+03	-1.571398929D+02	4.016322310D+00	1.743396078D-02	-2.252789060D-05				
1.433673443D-08	-3.648755580D-12		-7.822452620D+04	6.886094746D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								13230.913
-2.233613309D+05	-6.440602960D+02	1.047861848D+01	-1.911892367D-04	4.224887790D-08				
-4.847266920D-12	2.247974725D-16		-7.740626480D+04	-2.814630564D+01				

BFOH Gurvich,1996a pt1 p71 pt2 p48.

2 g 9/98 B	1.00F	1.000	1.00H	1.00	0.00	0	46.8167432	-451631.678
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11973.122
-7.563953670D+04	1.354838128D+03	-5.648210110D+00	3.870274660D-02	-5.037659180D-05				
3.339592640D-08	-8.847822950D-12		-6.194446110D+04	5.800362820D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11973.122
7.251318090D+05	-3.215620850D+03	1.117909777D+01	-1.883881929D-04	2.579708080D-09				
2.665158100D-12	-2.186647438D-16		-3.716808080D+04	-3.978463490D+01				

BF(OH)2 Gurvich,1996a pt1 p71 pt2 p49.

2 tpis96 B	1.00F	1.000	2.00H	2.00	0.00	0	63.8240832	-1049889.539
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12885.220
1.381800676D+04	2.529637004D+02	-3.844552040D+00	5.255140850D-02	-7.193117730D-05				
4.948309910D-08	-1.345922496D-11		-1.283123258D+05	4.293659370D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12885.220
1.422037640D+06	-6.257297570D+03	1.822460686D+01	-3.221396450D-04	-7.126739900D-09				
6.758699770D-12	-5.042554540D-16		-9.186254190D+04	-8.527895050D+01				

## Appendix D (continued)

BF2 Gurvich,1996a pt1 p58 pt2 p37.  
 2 tps96 B 1.00F 2.00 0.00 0.00 0.00 0 48.8078064 -499426.904  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10612.202  
 -6.787651760D+04 1.085903536D+03-3.023320961D+00 2.326503687D-02-2.641444147D-05  
 1.515620683D-08-3.518559180D-12 -6.640918250D+04 4.431968310D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10612.202  
 -1.153091296D+05-8.109800120D+02 7.602709230D+00-2.409209242D-04 5.328471860D-08  
 -6.118797940D-12 2.839984178D-16 -5.796222170D+04-1.655644047D+01  
 BF2+ Chase,1998 p211.  
 2 j12/70 B 1.00F 2.00E -1.00 0.00 0.00 0 48.8072578 322586.400  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10612.483  
 -2.938356477D+04 2.955698598D+02 1.894274526D+00 1.280508319D-02-1.388757254D-05  
 7.624366750D-09-1.706339371D-12 3.598992440D+04 1.384803311D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10612.483  
 -1.769409966D+05-5.343685180D+02 7.728052910D+00-1.958622052D-06-2.419680893D-08  
 5.732533810D-12-3.216354230D-16 3.908745050D+04-1.936560315D+01  
 BF2- Gurvich,1996a pt1 p60 pt2 p38.  
 2 tps96 B 1.00F 2.00E 1.00 0.00 0.00 0 48.8083550 -733802.963  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10433.571  
 2.109765318D+04 1.439564600D+02 2.604646296D-01 1.817373751D-02-2.241565287D-05  
 1.369712886D-08-3.355952680D-12 -8.971801780D+04 2.351692604D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10433.571  
 -1.709920627D+05-6.156219790D+02 7.458871370D+00-1.836703248D-04 4.064363960D-08  
 -4.667700950D-12 2.166264840D-16 -8.741404530D+04-1.620604664D+01  
 BF2CL Gurvich,1996a pt1 p87 pt2 p65.  
 2 tps96 B 1.00F 2.00CL 1.00 0.00 0.00 0 84.2608064 -888000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12323.693  
 4.500101250D+03-1.196284966D+02 3.198635140D+00 1.743426933D-02-1.994070287D-05  
 1.125136430D-08-2.544020371D-12 -1.076779851D+05 1.008195015D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12323.693  
 -2.066817398D+05-1.024447292D+03 1.075843981D+01-3.023235319D-04 6.672521470D-08  
 -7.649941900D-12 3.546224500D-16 -1.046936725D+05-3.229995036D+01  
 BF2OH Gurvich,1996a pt1 p72 pt2 p50.  
 2 tps96 B 1.00F 2.000 1.00H 1.00 0.00 0 65.8151464 -1092217.322  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12395.887  
 -7.522521650D+03 4.367121690D+02-3.128973474D+00 4.323957680D-02-5.785494040D-05  
 3.885858130D-08-1.038574523D-11 -1.344259458D+05 4.139170550D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12395.887  
 5.760759250D+05-3.611900190D+03 1.446897640D+01-3.028293733D-04 2.764337508D-08  
 -1.905493170D-13-8.694971940D-17 -1.133589041D+05-5.896981510D+01  
 BF3 Gurvich,1996a pt1 p62 pt2 p39.  
 2 tps96 B 1.00F 3.00 0.00 0.00 0.00 0 67.8062096 -1136000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11651.226  
 3.465584000D+03 2.133198651D+01 1.641245191D+00 1.993755064D-02-2.150119930D-05  
 1.145669081D-08-2.442285789D-12 -1.379455591D+05 1.625533544D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11651.226  
 -1.819767014D+05-1.405347931D+03 1.103412258D+01-4.104591050D-04 9.031277570D-08  
 -1.033057360D-11 4.780551830D-16 -1.323136863D+05-3.738386080D+01  
 BF4- Gurvich,1996a pt1 p63 pt2 p40.  
 2 tps96 B 1.00F 4.00E 1.00 0.00 0.00 0 86.8051614 -1761265.998  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13795.643  
 2.068485200D+05-2.463190805D+03 1.206414196D+01 1.102766923D-02-1.751720760D-05  
 1.201346256D-08-3.150588626D-12 -2.010569206D+05-4.610826940D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13795.643  
 -4.373241710D+05-7.759289410D+02 1.358222575D+01-2.341024178D-04 5.196915940D-08  
 -5.982245780D-12 2.781163206D-16 -2.127251877D+05-4.953369700D+01  
 BH Bauschlicher,1990. Gurvich,1996a pt1 p28 pt2 p19.  
 2 g12/99 B 1.00H 1.00 0.00 0.00 0.00 0 11.8189400 448727.204  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8639.104  
 2.063082550D+04-3.682502520D+02 6.071337870D+00-8.728321070D-03 1.458566459D-05  
 -1.036840401D-08 2.779462579D-12 5.460459920D+04-1.300392582D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8639.104  
 -1.098531663D+06-1.745890126D+02 8.442426810D+00-5.440196670D-03 2.718307052D-06  
 -4.839812210D-10 2.868523222D-14 5.016735670D+04-2.971030686D+01

## Appendix D (continued)

BHCL Gurvich,1996a pt1 p81 pt2 p58.  
 2 g 9/98 B 1.00H 1.00CL 1.00 0.00 0.00 0 47.2719400 141418.307  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10304.807  
 4.763274910D+04-4.420016520D+02 3.975645880D+00 8.541698760D-03-1.377785182D-05  
 1.131521587D-08-3.569659180D-12 1.822278428D+04 3.028452399D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10304.807  
 3.499991720D+05-2.238404757D+03 8.711106050D+00-1.088882906D-03 4.189301090D-07  
 -6.568711260D-11 3.620067600D-15 2.841240364D+04-2.589566225D+01

BHCL2 Gurvich,1996a pt1 p82 pt2 p60.  
 2 tpis96 B 1.00H 1.00CL 2.00 0.00 0.00 0 82.7249400 -251883.529  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11745.632  
 4.419914810D+04-2.384739577D+02 1.356682235D+00 2.517866897D-02-3.632910400D-05  
 2.644335581D-08-7.625044110D-12 -3.003877914D+04 1.787024616D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11745.632  
 4.110996060D+05-2.858027441D+03 1.179547506D+01-6.322817970D-04 1.269551549D-07  
 -1.352862344D-11 5.921653510D-16 -1.617288760D+04-4.217900972D+01

BHF Gurvich,1996a pt1 p68 pt2 p45.  
 2 g 9/98 B 1.00H 1.00F 1.00 0.00 0.00 0 30.8173432 -76012.343  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10042.057  
 -4.908362260D+04 9.610760210D+02-2.919850316D+00 2.149156633D-02-2.595677863D-05  
 1.693492714D-08-4.553648840D-12 -1.466925195D+04 4.160709310D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10042.057  
 1.184821300D+06-4.677435180D+03 1.067328148D+01-1.606366598D-03 3.704534700D-07  
 -3.797882750D-11 1.432441145D-15 1.802640937D+04-4.285931170D+01

BHFL Gurvich,1996a pt1 p90 pt2 p69.  
 2 tpis96 B 1.00H 1.00F 1.00CL 1.00 0.00 0 66.2703432 -483036.620  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11414.539  
 5.761169720D+02 3.042156250D+02-9.808900360D-01 2.803843648D-02-3.676734020D-05  
 2.499824138D-08-6.873421640D-12 -6.050207390D+04 3.132842092D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11414.539  
 4.390778920D+05-3.137181709D+03 1.200286161D+01-7.153669340D-04 1.453878608D-07  
 -1.565197070D-11 6.910075060D-16 -4.232368340D+04-4.466542881D+01

BHF2 Gurvich,1996a pt1 p69 pt2 p47.  
 2 tpis96 B 1.00H 1.00F 2.00 0.00 0.00 0 49.8157464 -739613.811  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10659.347  
 -8.353540280D+04 1.616659766D+03-8.161405670D+00 4.153786790D-02-4.921063280D-05  
 3.054165306D-08-7.786813980D-12 -9.748065460D+04 7.038630750D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10659.347  
 4.660876960D+05-3.728100490D+03 1.244152658D+01-8.906843190D-04 1.841732568D-07  
 -2.010774349D-11 8.979196590D-16 -6.978142930D+04-5.103218040D+01

BH2 Jacox,1994. Kolbuszewski,1996. Gurvich,1996a p32.  
 2 g 2/00 B 1.00H 2.00 0.00 0.00 0.00 0 12.8268800 328909.059  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10023.559  
 2.812557296D+04-3.000083489D+02 4.824221000D+00-2.186429819D-04 1.485457398D-06  
 3.893739680D-10-6.331629390D-13 3.991988420D+04-5.042682850D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10023.559  
 1.360117365D+06-4.917704490D+03 9.758971030D+00-7.415870640D-04 1.269760019D-07  
 -1.187742442D-11 4.682552510D-16 6.890292660D+04-4.190490120D+01

BH2CL Gurvich,1996a pt1 p82 pt2 p59.  
 2 tpis96 B 1.00H 2.00CL 1.00 0.00 0.00 0 48.2798800 -80845.754  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10426.902  
 1.646638117D+04 1.277320942D+02 1.300268921D-01 1.938143193D-02-2.316389616D-05  
 1.607896164D-08-4.668337650D-12 -1.112112215D+04 2.308500112D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10426.902  
 1.427215437D+06-6.265564340D+03 1.382183005D+01-1.313843556D-03 2.587131606D-07  
 -2.713845270D-11 1.172827257D-15 2.639387516D+04-6.399725308D+01

BH2F Gurvich,1996a pt1 p69 pt2 p46.  
 2 tpis96 B 1.00H 2.00F 1.00 0.00 0.00 0 31.8252832 -323956.732  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10137.922  
 -8.837920440D+04 1.705285929D+03-8.061246130D+00 3.643188680D-02-4.152482550D-05  
 2.620135756D-08-6.930886410D-12 -4.787273410D+04 6.862087670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10137.922  
 1.435082111D+06-6.625320170D+03 1.409165008D+01-1.422469060D-03 2.828724718D-07  
 -2.992498948D-11 1.302618926D-15 -7.937192670D+02-6.801356400D+01

## Appendix D (continued)

BH3 Allendorf,1997. Jacox,1998 p212. Martin,1992.

2 g 1/00 B	1.00H	3.00	0.00	0.00	0.00	0	13.8348200	104746.599
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.619635070D+04	1.262658391D+03	-4.654355900D+00	2.461795131D-02	-2.501537437D-05				
1.562330756D-08	-4.323949480D-12		5.667587980D+03	4.666504620D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.855778950D+06	-8.002492370D+03	1.505692199D+01	-1.790456689D-03	3.612511100D-07				
-3.866035910D-11	1.698508879D-15		5.967537070D+04	-7.994046160D+01				

BH3NH3 Gurvich,1996a pt1 p106 pt2 p84.

2 tpis96 B	1.00H	6.00N	1.00	0.00	0.00	0	30.8653400	-115000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.811063598D+05	3.010341543D+03	-1.524271135D+01	6.215637750D-02	-5.959881850D-05				
3.267429360D-08	-7.751243090D-12		-2.934278877D+04	1.087399608D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.354925960D+06	-1.824235232D+04	3.162999830D+01	-3.208243610D-03	5.885075450D-07				
-5.808535530D-11	2.382578600D-15		9.438118030D+04	-1.897865799D+02				

BH4 Radical. Saxon,1993. Yu,1998.

2 g 5/00 B	1.00H	4.00	0.00	0.00	0.00	0	14.8427600	255210.477
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.734274578D+04	-8.473619380D+01	1.551871695D+00	1.439765491D-02	-6.111152360D-06				
-1.324417559D-10	5.133008150D-13		3.022048074D+04	1.250358328D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.354714146D+06	-7.870762750D+03	1.826170610D+01	-1.948275329D-03	4.072706890D-07				
-4.482710900D-11	2.014115885D-15		7.470249490D+04	-9.686086890D+01				

BH5 Schreiner,1994.

2 g 8/00 B	1.00H	5.00	0.00	0.00	0.00	0	15.8507000	92933.658
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.603075360D+04	1.457641959D+03	-8.245037630D+00	4.817478230D-02	-5.535104700D-05				
3.578299590D-08	-9.717757500D-12		3.424238930D+03	6.695881520D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.472199159D+06	-1.110339842D+04	2.243395706D+01	-2.121632568D-03	4.038994240D-07				
-4.121910490D-11	1.741706383D-15		7.561744630D+04	-1.243306259D+02				

BI Gurvich,1996a pt1 p94 pt2 p73.

2 g 9/98 B	1.00I	1.00	0.00	0.00	0.00	0	137.7154700	325987.502
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.517449530D+04	-5.445819300D+02	6.027511010D+00	-2.387237926D-03	2.244796277D-06				
-1.110001347D-09	2.280204403D-13		4.071910130D+04	-7.288049840D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.132872626D+06	-6.283684960D+03	1.123964343D+01	-3.258856750D-03	7.064282150D-07				
-4.230068930D-11	-4.208078470D-16		7.797634810D+04	-4.664042610D+01				

BI2 Gurvich,1996a pt1 p95 pt2 p74.

2 g 9/98 B	1.00I	2.00	0.00	0.00	0.00	0	264.6199400	238096.324
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.640975900D+04	-1.044411994D+03	9.734197240D+00	-3.952557540D-03	3.165567780D-06				
-1.273764644D-09	1.879968132D-13		3.205750890D+04	-2.012407058D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.924022230D+05	4.422902350D+02	7.129623580D+00	-5.619634060D-04	3.180760520D-07				
-5.537079720D-11	3.183959700D-15		2.291972638D+04	-3.201793240D+00				

BI3 Gurvich,1996a pt1 p96 pt2 p75.

2 tpis96 B	1.00I	3.00	0.00	0.00	0.00	0	391.5244100	21400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.243114890D+04	-1.002408628D+03	1.106650075D+01	1.609588058D-03	-5.147250250D-06				
4.732514020D-09	-1.512999796D-12		5.160348150D+03	-2.420687643D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.506176506D+05	-8.167210610D+01	1.005937867D+01	-2.319396215D-05	5.01996730D-09				
-5.654349630D-13	2.580651348D-17		-4.261687910D+02	-1.617962779D+01				

BN Gurvich,1996a pt1 p104 pt2 p83.

2 g 9/98 B	1.00N	1.00	0.00	0.00	0.00	0	24.8177000	574726.408
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.569707580D+04	6.704286070D+02	3.615089080D-02	7.339487510D-03	-4.969033490D-06				
1.229031380D-09	6.340281520D-14		6.485465080D+04	2.539869896D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.276932705D+05	-1.025649298D+02	4.414586810D+00	2.561670989D-04	-1.612994942D-08				
-6.526052930D-13	5.749466120D-17		6.784465130D+04	-6.778568656D-01				

## Appendix D (continued)

BO Gurvich,1996a pt1 p10 pt2 p8.  
 3 g 9/98 B 1.000 1.00 0.00 0.00 0.00 0 26.8104000 20406.404  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8674.104  
 -1.166216822D+04 9.217579390D+01 3.655498490D+00-3.118542920D-03 9.008329830D-06  
 -8.017789990D-09 2.472952292D-12 8.738284780D+02 4.482847390D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8674.104  
 1.788600589D+04-6.309019630D+02 4.574528400D+00 1.988001643D-04-9.702963480D-08  
 1.870854291D-11-1.030218131D-15 4.841311090D+03-3.398890580D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8674.104  
 -1.592699514D+08 1.210955629D+05-3.136823502D+01 5.110037760D-03-3.461020740D-07  
 1.148046833D-11-1.504899225D-16 -9.345065760D+05 3.026123907D+02  
 BO- Gurvich,1996a pt1 p13 pt2 p10.  
 2 g 9/98 B 1.000 1.00E 1.00 0.00 0.00 0 26.8109486 -277791.076  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8674.024  
 -8.242023210D+04 9.203636900D+02-2.302659981D-01 6.229904120D-03-3.157624391D-06  
 1.184578107D-10 2.819228693D-13 -3.911141220D+04 2.599226838D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8674.024  
 2.122804369D+05-1.262124688D+03 5.383167310D+00-3.181049100D-04 7.288988250D-08  
 -8.141708920D-11-3.715364390D-16 -2.706892261D+04-9.773753670D+00  
 BOCL Gurvich,1996a pt1 p79 pt2 p55.  
 2 tps96 B 1.000 1.00CL 1.00 0.00 0.00 0 62.2634000 -318536.695  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10607.913  
 7.052380640D+04-1.315301429D+03 1.130087727D+01-1.207112050D-02 1.880516131D-05  
 -1.373823975D-08 3.854890160D-12 -3.355399100D+04-3.698462517D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10607.913  
 1.557148487D+05-1.446254968D+03 8.509448050D+00-3.859007380D-04 8.262268820D-08  
 -9.261027460D-12 4.219998010D-16 -3.203589040D+04-2.372713292D+01  
 BOCL2 Gurvich,1996a pt1 p79 pt2 p56.  
 2 tps96 B 1.000 1.00CL 2.00 0.00 0.00 0 97.7164000 -361565.512  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13169.650  
 7.322667360D+04-2.027726965D+02 4.161924090D+00 1.733309456D-02-2.263908718D-05  
 1.452275190D-08-3.719593120D-12 -4.414441880D+04 6.520424110D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13169.650  
 -2.297527041D+05-6.194567930D+02 1.046075518D+01-1.841620739D-04 4.071215430D-08  
 -4.672246550D-12 2.167237536D-16 -4.371538420D+04-2.743570215D+01  
 BOF Gurvich,1996a pt1 p65 pt2 p42.  
 2 tps96 B 1.000 1.00F 1.00 0.00 0.00 0 45.8088032 -592978.311  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9988.295  
 7.226802650D+04-1.131386630D+03 8.816054520D+00-4.627694570D-03 7.801299580D-06  
 -5.681205840D-09 1.534732094D-12 -6.711116010D+04-2.547957229D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9988.295  
 1.937020297D+05-1.739112297D+03 8.695650860D+00-4.518895570D-04 9.591019080D-08  
 -1.067806769D-11 4.840007660D-16 -6.330152390D+04-2.702458617D+01  
 BOF2 Gurvich,1996a pt1 p66 pt2 p43.  
 2 tps96 B 1.000 1.00F 2.00 0.00 0.00 0 64.8072064 -832767.700  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11611.458  
 7.22794130D+03 2.148783624D+01 1.157840301D+00 2.250585296D-02-2.610731536D-05  
 1.508824929D-08-3.518364850D-12 -1.013995733D+05 2.010127136D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11611.458  
 -2.205028861D+05-1.254238690D+03 1.092551380D+01-3.680144000D-04 8.107164940D-08  
 -9.281275060D-12 4.297549300D-16 -9.680447580D+04-3.482853330D+01  
 BOH Gurvich,1996a pt1 p41 pt2 p24.  
 2 tps96 B 1.000 1.00H 1.00 0.00 0.00 0 27.8183400 -6756.578  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10031.524  
 -7.521410270D+04 1.391444703D+03-5.630330180D+00 2.966358811D-02-3.830835180D-05  
 2.550606424D-08-6.795857210D-12 -8.341300280D+03 5.517690040D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10031.524  
 8.447498570D+05-3.016982887D+03 8.083864700D+00-1.609855388D-04-2.191830959D-09  
 3.127133119D-12-2.376665451D-16 1.647698495D+04-2.603227947D+01  
 BO2 Gurvich,1996a pt1 p14 pt2 p11.  
 2 g10/97 B 1.000 2.00 0.00 0.00 0.00 0 42.8098000 -309121.947  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10772.157  
 -4.141090640D+04 7.198854610D+02-1.477629435D+00 2.277415194D-02-2.786326934D-05  
 1.718462069D-08-4.278991440D-12 -4.177657690D+04 3.258458010D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10772.157  
 -3.834452340D+04-9.563261140D+02 8.200962780D+00-2.062130802D-04 9.872288990D-09  
 8.158366760D-12-7.527519660D-16 -3.423564020D+04-2.224772278D+01

## Appendix D (continued)

BO2- Gurvich,1996a pt1 p16 pt2 p13.  
 2 tps96 B 1.000 2.00E 1.00 0.00 0.00 0 42.8103486 -714493.991  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9597.541  
 5.324279690D+04-7.326313030D+02 5.902470000D+00 2.437465200D-03-4.878803950D-07  
 -8.475724760D-10 4.080781180D-13 -8.344293680D+04-1.053931911D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9597.541  
 1.199226372D+05-1.715766982D+03 8.701038220D+00-4.601242120D-04 9.867011870D-08  
 -1.107288516D-11 5.050183240D-16 -7.825789690D+04-2.839356505D+01

B(OH)2 Gurvich,1996a pt1 p46 pt2 p28.  
 2 g 9/98 B 1.000 2.00H 2.00 0.00 0.00 0 44.8256800 -425243.642  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11971.658  
 1.491659222D+03 3.648184840D+02-2.906006389D+00 4.136834460D-02-5.782584220D-05  
 4.069783560D-08-1.126499791D-11 -5.375483660D+04 3.88853180D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11971.658  
 1.557023406D+06-5.784710760D+03 1.487391235D+01-1.821804765D-04-3.803541640D-08  
 1.030332746D-11-6.685889830D-16 -1.806810301D+04-6.590268900D+01

BS Gurvich,1996a pt1 p97 pt2 p76.  
 2 g10/98 B 1.00S 1.00 0.00 0.00 0.00 0 42.8760000 273519.405  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8724.105  
 -3.839490100D+04 6.989417490D+02-1.213980460D+00 1.396391264D-02-1.689881284D-05  
 1.038889985D-08-2.582063989D-12 2.865685472D+04 3.154819945D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8724.105  
 1.358760165D+06-4.364035960D+03 9.034307590D+00-2.114548699D-03 4.189275310D-07  
 -1.354787322D-11-1.360684605D-15 5.913065450D+04-3.336696868D+01

BS2 Gurvich,1996a pt1 p99 pt2 p77.  
 2 g 9/98 B 1.00S 2.00 0.00 0.00 0.00 0 74.9410000 63867.460  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13559.560  
 1.820264374D+04-5.150671890D+02 8.547515000D+00-1.626155268D-03 1.866387194D-06  
 -1.277165468D-09 3.681980690D-13 8.186839750D+03-1.778384854D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13559.560  
 5.120402510D+05-1.938581076D+03 9.814873460D+00-1.339731606D-03 3.754301160D-07  
 -4.400383780D-11 1.887662968D-15 1.736535000D+04-2.757546712D+01

B2 Gurvich,1996a pt1 p8 pt2 p7.  
 2 g 9/98 B 2.00 0.00 0.00 0.00 0 21.6220000 857370.506  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8805.106  
 -1.516418096D+05 2.630168946D+03-1.381358321D+01 5.216225190D-02-6.930494740D-05  
 4.469410390D-08-1.128496456D-11 8.995251050D+04 9.813118490D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8805.106  
 1.094594495D+06-2.602735739D+03 6.909456210D+00-6.405949890D-04 1.951732355D-07  
 -2.555902119D-11 1.053557323D-15 1.187807611D+05-1.949045025D+01

B2C Gurvich,1996a pt1 p110 pt2 p88.  
 2 g 9/98 B 2.00C 1.00 0.00 0.00 0.00 0 33.6327000 800432.614  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11723.114  
 -4.166519870D+04 5.797779520D+02 1.411017091D+00 1.174705713D-02-1.066474425D-05  
 4.717232620D-09-7.970013260D-13 9.196874200D+04 1.769254387D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11723.114  
 1.159241019D+06-4.567798810D+03 1.228672097D+01-2.500830701D-03 6.409979850D-07  
 -6.932935770D-11 2.672933741D-15 1.222442137D+05-5.199066186D+01

B2CL4 Gurvich,1996a pt1 p77 pt2 p54.  
 2 g10/97 B 2.00CL 4.00 0.00 0.00 0.00 0 163.4340000 -490000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21588.132  
 4.285555130D+04-7.280748810D+02 9.315763670D+00 2.331629623D-02-3.511247610D-05  
 2.464057658D-08-6.735479960D-12 -5.819023240D+04-1.622083878D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21588.132  
 -6.427987030D+05 5.078562990D+02 1.486725022D+01 2.026983515D-06 6.272718810D-09  
 -1.218822573D-12 7.241208410D-17 -6.820066000D+04-4.139110669D+01

B2F4 Gurvich,1996a pt1 p64 pt2 p41.  
 2 g10/97 B 2.00F 4.00 0.00 0.00 0.00 0 97.6156128 -1438000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17680.793  
 -5.971695640D+04 8.189425440D+02-6.437671290D-01 3.858966070D-02-4.313053190D-05  
 2.404463223D-08-5.393559350D-12 -1.790041225D+05 3.552179970D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17680.793  
 3.855865890D+04-2.928842655D+03 1.792063736D+01-9.523998270D-04 1.614708845D-07  
 -1.428613504D-11 5.218739670D-16 -1.613051924D+05-7.184803250D+01

## Appendix D (continued)

B2H Adams, 1989. Yu, 1998.

2 g 7/00 B	2.00H	1.00	0.00	0.00	0.00	0	22.6299400	796262.497
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.775579740D+04	-1.343931564D+03	9.832099150D+00	-5.607137750D-03	5.730651050D-06				
-2.266436197D-09	1.972352080D-13		1.009908698D+05	-3.282461480D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.175545750D+05	-2.627897466D+03	9.084905070D+00	-5.389418330D-04	1.050714700D-07				
-1.092459556D-11	4.684854660D-16		1.099537555D+05	-3.164029910D+01				

B2H2 Curtiss, 1989a. Yu, 1998.

2 g 7/00 B	2.00H	2.00	0.00	0.00	0.00	0	23.6378800	454677.939
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.421617322D+05	-2.138011262D+03	1.317732399D+01	-8.942658070D-03	1.127804935D-05				
-5.787886200D-09	1.000813871D-12		6.372319250D+04	-5.346982740D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.240614592D+06	-5.368965020D+03	1.379292454D+01	-1.136749748D-03	2.245617156D-07				
-2.361530467D-11	1.022604572D-15		8.506511490D+04	-6.435461300D+01				

B2H3 Adams, 1989. Yu, 1998.

2 g 6/00 B	2.00H	3.00	0.00	0.00	0.00	0	24.6458200	351072.721
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.425147160D+04	-1.075866284D+03	6.383999390D+00	1.167858327D-02	-1.429661252D-05				
1.128776882D-08	-3.681325060D-12		4.635335080D+04	-1.400002845D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.771506902D+06	-7.872260930D+03	1.789447015D+01	-1.709304785D-03	3.409575430D-07				
-3.614543680D-11	1.575671409D-15		8.737711890D+04	-9.054629460D+01				

B2H3,db 2-Bridges. Adams, 1989. Yu, 1998.

2 g 7/00 B	2.00H	3.00	0.00	0.00	0.00	0	24.6458200	353408.227
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.064014840D+04	-7.524466330D+02	5.584483840D+00	1.080468494D-02	-8.649032810D-06				
4.748333310D-09	-1.309096028D-12		4.491792300D+04	-8.873686820D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.497731017D+06	-7.219314140D+03	1.750463766D+01	-1.579698800D-03	3.164103470D-07				
-3.367225150D-11	1.472919654D-15		8.324349670D+04	-8.779549260D+01				

B2H4 1-Bridge. Ruscic, 1989b. Curtiss, 1989b.

2 g 8/00 B	2.00H	4.00	0.00	0.00	0.00	0	25.6537600	211162.059
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.000132300D+04	-3.071548876D+02	1.763071673D+00	2.646361882D-02	-3.066168202D-05				
2.163781936D-08	-6.491835410D-12		2.581033714D+04	1.015267130D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.292078842D+06	-1.059832517D+04	2.268612155D+01	-2.363586598D-03	4.762173070D-07				
-5.090100400D-11	2.233911590D-15		8.638591980D+04	-1.246794566D+02				

B2H4,db 2-Bridges. Ruscic, 1989b. Curtiss, 1989b.

2 g 7/00 B	2.00H	4.00	0.00	0.00	0.00	0	25.6537600	209932.448
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.781496923D+04	5.716048040D+02	-2.763085348D+00	3.125348696D-02	-2.709524346D-05				
1.341728634D-08	-3.004352798D-12		2.158138307D+04	3.675872940D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.886854256D+06	-1.010045614D+04	2.247110812D+01	-2.319968667D-03	4.731879960D-07				
-5.110673030D-11	2.262693782D-15		8.233487000D+04	-1.237455797D+02				

B2H5 1-Bridge. Ruscic, 1989a. Trachtman, 1989.

2 g 5/00 B	2.00H	5.00	0.00	0.00	0.00	0	26.6617000	254783.889
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.830965450D+04	-4.066148050D+01	-1.422523787D+00	3.674595270D-02	-3.851989710D-05				
2.444494440D-08	-6.821722940D-12		3.008956452D+04	2.802425895D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.696691012D+06	-1.320019835D+04	2.735260413D+01	-2.961879012D-03	5.984999430D-07				
-6.413748550D-11	2.821187823D-15		1.064524901D+05	-1.559654379D+02				

B2H5,db 2-Bridges. Ruscic, 1989a. Trachtman, 1989.

2 g 5/00 B	2.00H	5.00	0.00	0.00	0.00	0	26.6617000	275150.616
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.424446027D+04	4.204558200D+02	-3.700451250D+00	3.672053100D-02	-3.193503730D-05				
1.695013434D-08	-4.257038140D-12		3.046684683D+04	4.245495820D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.571729448D+06	-1.356829858D+04	2.781376038D+01	-3.192365030D-03	6.561165260D-07				
-7.127333940D-11	3.169492650D-15		1.106370527D+05	-1.597214457D+02				

## Appendix D (continued)

B2H6 Hf:Gurvich,1996a pt1 p37. Yu,1998. Duncan,1985.  
 2 g 5/00 B 2.00H 6.00 0.00 0.00 0.00 0 27.6696400 36600.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11932.313  
 -1.052844558D+04 1.041795556D+03-8.960518860D+00 5.492480880D-02-5.305197050D-05  
 3.011904756D-08-7.688768300D-12 -9.259374350D+02 6.812592430D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11932.313  
 2.835765414D+06-1.567600163D+04 3.226122330D+01-3.738609730D-03 7.718806460D-07  
 -8.414454540D-11 3.752223380D-15 9.358378550D+04-1.920223395D+02

B2O Gurvich,1996a pt1 p19 pt2 p14.  
 2 g 9/98 B 2.000 1.00 0.00 0.00 0.00 0 37.6214000 192798.018  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11783.018  
 -5.699546760D+04 1.018000465D+03-2.636481947D+00 2.746009279D-02-3.632432720D-05  
 2.406890217D-08-6.384129720D-12 1.703874394D+04 3.855346110D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11783.018  
 -1.628723220D+05-3.876289810D+02 7.787723520D+00-1.146822108D-04 2.528097612D-08  
 -2.893783941D-12 1.339210475D-16 2.263035354D+04-1.908513011D+01

B2O2 Gurvich,1996a pt1 p19 pt2 p15.  
 2 tpis96 B 2.000 2.00 0.00 0.00 0.00 0 53.6208000 -457711.486  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13396.618  
 8.174391690D+04-1.732702797D+03 1.605560926D+01-2.160057288D-02 3.566854570D-05  
 -2.660198794D-08 7.531833240D-12 -4.899632900D+04-6.172702390D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13396.618  
 4.605789660D+05-2.990079203D+03 1.256764079D+01-7.850974950D-04 1.672537624D-07  
 -1.867694780D-11 8.486190670D-16 -4.015748150D+04-4.874413710D+01

B2O3 Gurvich,1996a pt1 p25 pt2 p18.  
 2 tpis96 B 2.000 3.00 0.00 0.00 0.00 0 69.6202000 -835382.271  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14418.729  
 7.379611910D+04-1.263620592D+03 1.072681512D+01 3.841383720D-04 5.976058380D-06  
 -6.552891350D-09 2.123951064D-12 -9.628183140D+04-3.088078011D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14418.729  
 3.905035300D+05-3.691348210D+03 1.555502598D+01-9.707645510D-04 2.068887872D-07  
 -2.310858356D-11 1.050136734D-15 -8.263054410D+04-6.390863440D+01

B2(OH)4 Gurvich,1996a pt1 p52 pt2 p33.  
 2 g 9/98 B 2.000 4.00H 4.00 0.00 0.00 0 89.6513600 -1254987.531  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19443.069  
 -1.728717249D+04 8.495913480D+02-8.715959570D+00 9.362362610D-02-1.278784165D-04  
 8.813671160D-08-2.400605571D-11 -1.564337133D+05 7.120169310D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19443.069  
 2.983925656D+06-1.207469577D+04 3.162610570D+01-5.163682440D-04-4.232093970D-08  
 1.671977280D-11-1.156366726D-15 -8.280976970D+04-1.653010498D+02

B2S Gurvich,1996a pt1 p100, pt2 p78.  
 2 g 9/98 B 2.00S 1.00 0.00 0.00 0.00 0 53.6870000 622260.705  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13182.705  
 6.638609300D+04-9.201185690D+02 8.699831340D+00 7.645589010D-04-3.709026030D-06  
 3.642373980D-09-1.197766071D-12 7.770375800D+04-2.251712444D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13182.705  
 -1.211501483D+05-6.473398450D+01 7.546825610D+00-1.820541450D-05 3.923951170D-09  
 -4.403862380D-13 2.003651718D-17 7.258531870D+04-1.394971229D+01

B2S2 Gurvich,1996a pt1 p100 pt2 p79.  
 2 tpis96 B 2.00S 2.00 0.00 0.00 0.00 0 85.7520000 138317.112  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14569.112  
 -7.061549970D+04 7.182944780D+02 1.919797788D+00 2.036407461D-02-2.309813846D-05  
 1.311616725D-08-2.996394781D-12 1.100829019D+04 1.855402586D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14569.112  
 -1.641535014D+05-7.742865640D+02 1.107731737D+01-2.313278554D-04 5.125614290D-08  
 -5.894081230D-12 2.738673834D-16 1.733003515D+04-3.359766998D+01

B2S3 Gurvich,1996a pt1 p102 pt2 p81.  
 2 tpis96 B 2.00S 3.00 0.00 0.00 0.00 0 117.8170000 17754.057  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19938.057  
 -3.431268500D+04 5.587615370D+02 3.414077410D+00 2.398333891D-02-2.841617637D-05  
 1.690005199D-08-4.060070710D-12 -3.027690575D+03 1.846767864D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19938.057  
 -1.905855086D+05-9.348342480D+02 1.369333613D+01-2.766647250D-04 6.110155800D-08  
 -7.008048570D-12 3.249524620D-16 2.906433760D+03-3.946870479D+01



## Appendix D (continued)

B3H7, C2v C2v symmetry. Stanton, 1989b.

2 g 8/00 B	3.00H	7.00	0.00	0.00	0.00	0	39.4885800	176019.139
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.086009469D+05	-7.921536800D+02	-9.577368040D-01	5.656119290D-02	-6.405034500D-05				
4.281322960D-08	-1.227580455D-11		2.430638819D+04	2.102582666D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.598592140D+06	-1.863701968D+04	3.993998830D+01	-4.275410160D-03	8.705358820D-07				
-9.385105020D-11	4.147865310D-15		1.272154092D+05	-2.379769856D+02				

B3H7, Cs Cs symmetry. Stanton, 1989b.

2 g 8/00 B	3.00H	7.00	0.00	0.00	0.00	0	39.4885800	159318.322
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.298169330D+04	4.071745370D+02	-9.635730530D+00	7.944312000D-02	-9.306456820D-05				
6.105147350D-08	-1.685927691D-11		1.707069083D+04	6.873966560D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.281576450D+06	-1.811096595D+04	3.963832460D+01	-4.178424110D-03	8.526829060D-07				
-9.209600240D-11	4.076496770D-15		1.213622564D+05	-2.357090217D+02				

B3H9 Hf:McKee, 1990. Stanton, 1989a.

2 g 7/00 B	3.00H	9.00	0.00	0.00	0.00	0	41.5044600	138908.800
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.483214900D+04	-5.206163040D+02	-4.665701210D-01	5.346983860D-02	-4.155796820D-05				
1.944135439D-08	-4.541227350D-12		1.805101100D+04	2.110804198D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.863999500D+06	-2.229433407D+04	4.875046150D+01	-5.418449260D-03	1.125767651D-06				
-1.233226406D-10	5.520348180D-15		1.422187123D+05	-2.958240102D+02				

B3N3H6 Borazole. Gurvich, 1996a pt1 p107 pt2 p85.

2 tpis96 B	3.00N	3.00H	6.00	0.00	0.00	0	80.5007400	-512000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.552621082D+05	4.010211270D+03	-3.382491300D+01	1.624575582D-01	-2.065528647D-04				
1.368862991D-07	-3.673470900D-11		-8.051253400D+04	1.995000751D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.739245170D+06	-1.941238951D+04	4.445070030D+01	-3.210308050D-03	5.717465420D-07				
-5.486692140D-11	2.191943197D-15		4.758426160D+04	-2.641156625D+02				

B3O3CL3 Gurvich, 1996a pt1 p80 pt2 p57.

2 tpis96 B	3.00O	3.00CL	3.00	0.00	0.00	0	186.7902000	-1635982.041
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.284452800D+04	1.005623966D+03	-4.556519630D+00	8.117967140D-02	-1.038385803D-04				
6.621422330D-08	-1.695748504D-11		-2.040907277D+05	5.466113803D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.414059810D+05	-2.527447455D+03	2.687263667D+01	-7.463389360D-04	1.646334110D-07				
-1.886231553D-11	8.737926310D-16		-1.923509858D+05	-1.185636255D+02				

B3O3FCL2 Gurvich, 1996a pt1 p89 pt2 p68.

2 tpis96 B	3.00O	3.00F	1.00CL	2.00	0.00	0	170.3356032	-1883807.681
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.719120070D+04	8.673745890D+02	-4.095778460D+00	7.815563970D-02	-9.767035170D-05				
6.097610090D-08	-1.532880319D-11		-2.331383552D+05	5.198088158D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.162360830D+05	-2.851210308D+03	2.710953133D+01	-8.400919640D-04	1.852318684D-07				
-2.121694694D-11	9.827291560D-16		-2.202729252D+05	-1.210679365D+02				

B3O3F2CL Gurvich, 1996a pt1 p89 pt2 p67.

2 tpis96 B	3.00O	3.00F	2.00CL	1.00	0.00	0	153.8810064	-2132816.827
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.277015540D+04	1.104904696D+03	-5.854181050D+00	7.953943100D-02	-9.592660770D-05				
5.799856310D-08	-1.416698348D-11		-2.640400115D+05	6.071247222D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.810787490D+05	-3.370009020D+03	2.748953579D+01	-9.905442560D-04	2.182908440D-07				
-2.499573480D-11	1.157532106D-15		-2.472114785D+05	-1.261501548D+02				

B3O3F3 Gurvich, 1996a pt1 p67 pt2 p44.

2 tpis96 B	3.00O	3.00F	3.00	0.00	0.00	0	137.4264096	-2382699.078
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.251549780D+04	1.400996228D+03	-7.906716200D+00	8.217161850D-02	-9.633152660D-05				
5.668194260D-08	-1.349024305D-11		-2.953461728D+05	7.001536830D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.629822910D+05	-3.784946870D+03	2.779526578D+01	-1.112096232D-03	2.450806704D-07				
-2.806484980D-11	1.299750466D-15		-2.748865475D+05	-1.315605015D+02				

## Appendix D (continued)

B4H4 Yu,1998. Mach,1994.  
 2 g 8/00 B 4.00H 4.00 0.00 0.00 0.00 0 47.2757600 326190.400  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14936.602  
 2.171791579D+05-2.598282557D+03 9.845440610D+00 3.026309140D-02-4.128334160D-05  
 3.089368344D-08-9.353384260D-12 5.079143480D+04-3.770757210D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14936.602  
 1.937200886D+06-1.078185932D+04 2.879625241D+01-2.401547707D-03 4.837756780D-07  
 -5.170490230D-11 2.269138182D-15 9.836595390D+04-1.561814117D+02  
 B4H10 Wagman,1982 p123. McKee,1990. Dain,1981.  
 2 g 5/00 B 4.00H 10.00 0.00 0.00 0.00 0 53.3234000 66100.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15485.574  
 -3.296604820D+04 2.440532922D+03-2.685332563D+01 1.406499347D-01-1.586710574D-04  
 9.874594130D-08-2.601426018D-11 -3.091924018D+03 1.589905532D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15485.574  
 4.030474130D+06-3.250629762D+04 5.687233660D+01-6.178567860D-03 1.280621032D-06  
 -1.400254585D-10 6.258866560D-15 1.506009087D+05-3.520714200D+02  
 B4H12 Shen,1993. Yu,1998.  
 2 g 5/00 B 4.00H 12.00 0.00 0.00 0.00 0 55.3392800 188236.114  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21748.714  
 7.152170300D+04-1.590351575D+02-4.719771660D+00 8.811228900D-02-8.604946880D-05  
 5.123535510D-08-1.379865250D-11 2.194186547D+04 4.187897400D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21748.714  
 6.158360800D+06-2.202086730D+04 6.660443600D+01-7.406369280D-03 1.512993908D-06  
 -1.635619071D-10 7.245385140D-15 2.054586275D+05-4.142106860D+02  
 B5H9 Hf:Chase,1998 p303 3/65.McKee,1990.Beaudet,1988.Yu,1998.  
 2 g 6/00 B 5.00H 9.00 0.00 0.00 0.00 0 63.1264600 73220.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16052.677  
 8.998473720D+04 1.042533357D+02-1.195549834D+01 1.007310686D-01-9.866680210D-05  
 5.295535180D-08-1.232119583D-11 8.374341780D+03 7.663090480D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16052.677  
 3.169017620D+06-2.282503203D+04 5.512008980D+01-5.563411420D-03 1.157837073D-06  
 -1.270332301D-10 5.694262030D-15 1.334452571D+05-3.371060460D+02  
 Ba Gurvich,1996. Moore,1971. Moore,1970a. Gordon,1999.  
 3 g10/97 BA 1.00 0.00 0.00 0.00 0.00 0 137.3270000 185000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 2.222563526D+03-3.407977850D+01 2.706751118D+00-6.382894490D-04 1.063003846D-06  
 -9.102624270D-10 3.148062219D-13 2.166549702D+04 5.102545880D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 -1.926579228D+07 6.006501040D+04-6.633964130D+01 3.507565930D-02-7.807601830D-06  
 8.085126800D-10-3.199486918D-14 -3.589663720D+05 5.007583400D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 3.483452070D+08-2.925558261D+05 9.774888490D+01-1.345477126D-02 9.567239790D-07  
 -3.380662310D-11 4.727390540D-16 2.250335260D+06-7.968444410D+02  
 Ba+ Moore,1971. Gordon,1999.  
 3 g10/97 BA 1.00E -1.00 0.00 0.00 0.00 0 137.3264514 694049.528  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 -5.423167550D+04 6.744680780D+02-8.940272500D-01 8.796642950D-03-1.222812901D-05  
 8.387953870D-09-2.037964358D-12 7.941774640D+04 2.607063698D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 8.794971850D+06-1.951817883D+04 1.485542861D+01-9.404233500D-04-7.031257790D-07  
 1.667412753D-10-1.070117310D-14 2.146800732D+05-9.228264190D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 -1.055569557D+08 4.530799570D+04-5.410673220D-01-7.531497600D-04 1.295568595D-07  
 -6.013388590D-12 8.846178515D-17 -3.000874708D+05 4.370610780D+01  
 BaBr Gurvich,1996a pt1 p576 pt2 p437.  
 2 tpis96 BA 1.00BR 1.00 0.00 0.00 0.00 0 217.2310000 -75324.677  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10200.123  
 -6.912557440D+02-6.245500160D+01 4.796677650D+00-6.838004940D-04 1.043947680D-06  
 -7.441224300D-10 2.172187003D-13 -1.011349165D+04 5.196454870D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10200.123  
 -1.056014042D+06 1.034740207D+03 6.735729380D+00-3.784026300D-03 1.952196896D-06  
 -3.347831880D-10 1.893189803D-14 -1.950233645D+04-5.069279640D+00  
 BaBr2 Gurvich,1996a pt1 p579 pt2 p439.  
 2 tpis96 BA 1.00BR 2.00 0.00 0.00 0.00 0 297.1350000 -412514.741  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15485.759  
 -5.143374060D+03-3.870518460D+01 7.162446970D+00-3.696715310D-04 4.689715270D-07  
 -3.107902475D-10 8.363582050D-14 -5.153318260D+04 9.741407000D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15485.759  
 -8.928251210D+03-7.536558890D-01 7.000658210D+00-2.949821710D-07 7.092392110D-11  
 -8.670038100D-15 4.221742310D-19 -5.172669490D+04 1.910185706D+00

## Appendix D (continued)

BaCL Gurvich,1996a pt1 p570 pt2 p433.  
 2 tps96 BA 1.00CL 1.00 0.00 0.00 0.00 0 172.7800000 -136290.881  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9877.119  
 -2.661946867D+03-7.724996340D+01 4.746106050D+00-3.523548880D-04 3.999198350D-07  
 -1.936413749D-10 4.124048530D-14 -1.736328141D+04 3.904455084D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9877.119  
 -1.075410089D+06 1.209303069D+03 6.272558600D+00-3.288110310D-03 1.717751087D-06  
 -2.910607065D-10 1.632658438D-14 -2.779173737D+04-3.574185216D+00

BaCL+ Gurvich,1996a pt1 p572 pt2 p434.  
 2 g12/97 BA 1.00CL 1.00E -1.00 0.00 0.00 0 172.7794514 348697.630  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9668.230  
 -8.951556690D+02-1.334692684D+02 4.935416120D+00-7.574054510D-04 8.355724000D-07  
 -4.685258510D-10 1.095343103D-13 4.125155990D+04 1.896278378D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9668.230  
 -1.829198157D+04-2.931616688D+00 4.502280710D+00 3.671788490D-05 2.396147871D-09  
 5.479458600D-14 1.174342316D-18 4.055100150D+04 4.503765564D+00

BaCL2 Gurvich,1996a pt1 p575 pt2 p436.  
 2 tps96 BA 1.00CL 2.00 0.00 0.00 0.00 0 208.2330000 -499301.387  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14599.113  
 -1.157501999D+03-2.054518828D+02 7.837514050D+00-1.867700704D-03 2.335378734D-06  
 -1.531373341D-09 4.088525090D-13 -6.115665280D+04-5.978149218D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14599.113  
 -2.216598768D+04-4.002483810D+00 7.003426740D+00-1.515820808D-06 3.611849210D-10  
 -4.386759060D-14 2.125803293D-18 -6.219095270D+04-1.132439694D+00

BaF Gurvich,1996a pt1 p562 pt2 p429.  
 2 tps96 BA 1.00F 1.00 0.00 0.00 0.00 0 156.3254032 -318993.788  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9342.112  
 2.530317292D+04-4.716995100D+02 6.185036220D+00-3.366678800D-03 4.011834560D-06  
 -2.506578601D-09 6.477258160D-13 -3.731872140D+04-6.220715380D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9342.112  
 1.868380434D+06-7.071099600D+03 1.466959284D+01-6.995950200D-03 2.366313845D-06  
 -3.287734300D-10 1.647896238D-14 3.571780680D+03-6.662390920D+01

BaF+ Gurvich,1996a pt1 p566 pt2 p430.  
 2 g12/97 BA 1.00F 1.00E -1.00 0.00 0.00 0 156.3248546 134063.214  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9201.714  
 2.840719922D+04-4.863571820D+02 5.946058390D+00-2.429844077D-03 2.445346729D-06  
 -1.316757471D-09 2.974886320D-13 1.730639076D+04-5.951206930D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9201.714  
 -4.054423670D+04-1.701997704D+01 4.513055340D+00 2.632753508D-05 2.612088236D-09  
 -9.502197930D-14 6.515176160D-18 1.474486570D+04 2.783167711D+00

BaF2 Gurvich,1996a pt1 p569 pt2 p432.  
 2 tps96 BA 1.00F 2.00 0.00 0.00 0.00 0 175.3238064 -812003.483  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13437.017  
 3.488395520D+04-7.648459560D+02 9.797750380D+00-5.756457510D-03 6.775603800D-06  
 -4.243614750D-09 1.093687692D-12 -9.590356450D+04-2.082035292D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13437.017  
 -5.508633660D+04-1.691114228D+01 7.013564880D+00-5.731909770D-06 1.321203959D-09  
 -1.565528167D-13 7.444983020D-18 -9.983529700D+04-4.389581490D+00

BaH Gurvich,1996a pt1 p554 pt2 p423.  
 2 tps96 BA 1.00H 1.00 0.00 0.00 0.00 0 138.3349400 209535.105  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8731.105  
 -3.765268880D+04 6.986680120D+02-1.313524351D+00 1.460648882D-02-1.802974829D-05  
 1.133031115D-08-2.865589059D-12 2.097478889D+04 3.230802600D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8731.105  
 -6.755466570D+06 1.730700212D+04-1.136812458D+01 5.617744740D-03-3.180788850D-07  
 -1.052342502D-10 1.111101879D-14 -8.954070380D+04 1.182377538D+02

BaI Gurvich,1996a pt1 p581 pt2 p440.  
 2 tps96 BA 1.00I 1.00 0.00 0.00 0.00 0 264.2314700 -10237.675  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10397.125  
 -4.186285540D+03 1.033094613D+01 4.428900230D+00 3.026019976D-04-2.591429408D-07  
 1.741605400D-10-3.370062760D-14 -2.636169733D+03 8.201924680D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10397.125  
 -3.533859660D+06 7.394258000D+03 1.285151488D+00-2.303429302D-03 2.214839289D-06  
 -4.681096810D-10 3.011371472D-14 -5.340229590D+04 3.710443870D+01

## Appendix D (continued)

BaI2                      Gurvich,1996a pt1 p584 pt2 p442.

2 tps96 BA	1.00I	2.00	0.00	0.00	0.00	0	391.1359400	-288439.965
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15790.435
-4.241592730D+03	-1.862214382D+01	7.078556750D+00	-1.793922821D-04	2.281437677D-07				
-1.514647881D-10	4.081498360D-14		-3.670351490D+04	3.163138970D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15790.435
-6.048224800D+03	-3.622729450D-01	7.000317450D+00	-1.425793502D-07	3.433349420D-11				
-4.201754980D-15	2.047703474D-19		-3.679650750D+04	3.615475320D+00				

BaO                      Gurvich,1996a pt1 p550 pt2 p419.

3 tps96 BA	1.00O	1.00	0.00	0.00	0.00	0	153.3264000	-117948.392
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9014.108
3.764398500D+04	-5.071555300D+02	5.392847280D+00	-4.119324690D-04	-6.527896620D-07				
9.430588420D-10	-3.436603030D-13		-1.275552614D+04	-3.752213760D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9014.108
1.318481698D+07	-3.854253250D+04	4.686741610D+01	-2.188646633D-02	5.335677450D-06				
-5.152304300D-10	1.433083400D-14		2.306902396D+05	-3.028332772D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9014.108
-1.104748482D+09	3.561451690D+05	-1.236258085D+01	-2.812895475D-03	3.310897210D-07				
-1.254960778D-11	1.696392420D-16		-3.157682531D+06	2.067297489D+02				

BaO+                      Gurvich,1996a pt1 p552 pt2 p421.

3 g11/98 BA	1.00O	1.00E	-1.00	0.00	0.00	0	153.3258514	511704.686
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9469.786
3.566410970D+05	-3.779246710D+03	1.673544137D+01	-1.306611610D-02	2.686157445D-06				
4.044077950D-09	-2.016508813D-12		7.983268490D+04	-7.285118550D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9469.786
-3.317679230D+05	1.594253495D+03	3.227247810D+00	5.722641500D-04	-1.147415658D-07				
1.382873231D-11	-6.384437030D-16		5.025247610D+04	1.409092365D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9469.786
-3.283193020D+06	2.046049762D+03	4.048225140D+00	9.872145390D-05	7.763808620D-11				
2.536329860D-13	-1.334411326D-18		4.456858530D+04	8.528620900D+00				

BaOH                      Gurvich,1996a pt1 p557 pt2 p425.

2 tps96 BA	1.00O	1.00H	1.00	0.00	0.00	0	154.3343400	-224256.513
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11224.581
3.776231510D+04	-8.891390220D+02	9.531718000D+00	-5.458825900D-03	4.941783010D-06				
-1.809327537D-09	2.050048305D-13		-2.441852965D+04	-2.489410158D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11224.581
2.637336694D+06	-8.365410400D+03	1.599803975D+01	-5.098446050D-03	1.594657431D-06				
-2.180478542D-10	1.084610688D-14		2.393550647D+04	-7.490705790D+01				

BaOH+                      Gurvich,1996a pt1 p558 pt2 p426.

2 tps96 BA	1.00O	1.00H	1.00E	-1.00	0.00	0	154.3337914	202019.313
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11302.980
2.797632165D+04	-7.680769400D+02	9.052978440D+00	-4.368577900D-03	3.523497260D-06				
-8.386360870D-10	-6.475457470D-14		2.623280802D+04	-2.264561641D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11302.980
8.766738430D+05	-2.335819600D+03	7.973166060D+00	1.038679898D-04	-6.319485780D-08				
1.028729445D-11	-5.741808570D-16		3.772517470D+04	-1.930805001D+01				

Ba(OH)2                      Gurvich,1996a pt1 p561 pt2 p428.

2 tps96 BA	1.00O	2.00H	2.00	0.00	0.00	0	171.3416800	-606666.472
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								17388.725
5.702814900D+04	-1.577384797D+03	1.659935325D+01	-1.039598275D-02	9.664889600D-06				
-3.673621440D-09	4.625784990D-13		-6.835158900D+04	-5.851911700D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								17388.725
1.762908112D+06	-4.676205420D+03	1.395135494D+01	2.051842928D-04	-1.257265530D-07				
2.048917625D-11	-1.144045777D-15		-4.545964410D+04	-4.929457190D+01				

BaS                      Gurvich,1996a pt1 p585 pt2 p444.

2 tps96 BA	1.00S	1.00	0.00	0.00	0.00	0	169.3920000	38871.315
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9556.115
1.377075147D+04	-3.293500560D+02	5.811545840D+00	-2.848973760D-03	3.576336020D-06				
-2.325649347D-09	6.172805310D-13		4.964432450D+03	-3.497962615D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9556.115
6.104262070D+06	-2.227617479D+04	3.597513510D+01	-2.157793740D-02	7.319872350D-06				
-1.089038636D-09	5.884101950D-14		1.404138006D+05	-2.141776331D+02				

Ba2                      Gurvich,1996a pt1 p545 pt2 p417.

2 tps96 BA	2.00	0.00	0.00	0.00	0.00	0	274.6540000	355964.337
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11359.137
-1.294177083D+04	-7.276330080D+02	1.464866569D+01	-3.966331650D-02	5.898711060D-05				
-4.235300560D-08	1.189594362D-11		4.386712230D+04	-4.145673670D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11359.137
2.160114547D+05	1.950676877D+02	2.253699771D+00	1.507750613D-04	-4.742515000D-08				
7.048951960D-12	-3.547440170D-16		4.167762970D+04	2.375906459D+01				

## Appendix D (continued)

Be Hf:Cox,1989. Kramida,1997. Gordon,1999.

3 g11/97 BE	1.00	0.00	0.00	0.00	0.00	0	9.0121820	324000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

-4.112901520D-04 5.364967360D-06 2.499999972D+00 7.569203690D-11-1.097852652D-13

8.002110240D-17	-2.303022777D-20						3.822264590D+04	2.146172983D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

-6.926285840D+05 2.466773005D+03-9.776613340D-01 2.458939515D-03-9.047950420D-07

1.587880407D-10	-9.415600603D-15						2.300212917D+04	2.623234754D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

4.145833520D+08-2.254147519D+05 4.411437910D+01-3.022853591D-03 1.178346131D-07

-2.273387650D-12	1.196838345D-17						1.866686325D+06	-3.752337400D+02
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Be+ Moore,1971. Moore,1970a. Gordon,1999.

3 g 1/98 BE	1.00E	-1.00	0.00	0.00	0.00	0	9.0116334	1229701.328
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00

0.000000000D+00	0.000000000D+00						1.471528569D+05	2.839228698D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

-9.478135980D+04 2.768325398D+02 2.191388413D+00 1.648824289D-04-4.280166820D-08

4.542350470D-12	-6.270417825D-17						1.453850986D+05	5.055503840D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

-2.321269508D+08 1.525464518D+05-3.651092580D+01 4.812692090D-03-2.928878120D-07

8.899649840D-12	-1.055676610D-16						-1.052744318D+06	3.402173130D+02
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Be++ Moore,1970a. Gordon,1999.

3 g 3/97 BE	1.00E	-2.00	0.00	0.00	0.00	0	9.0110848	2993001.528
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00

0.000000000D+00	0.000000000D+00						3.592279160D+05	2.145990203D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00

0.000000000D+00	0.000000000D+00						3.592279160D+05	2.145990203D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6197.428

0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00

0.000000000D+00	0.000000000D+00						3.592279160D+05	2.145990203D+00
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BeBr Gurvich,1996a pt1 p374 pt2 p300.

2 tpis96 BE	1.00BR	1.00	0.00	0.00	0.00	0	88.9161820	132446.308
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8971.108

3.746288060D+04-4.722339070D+02 5.039409040D+00 5.798853220D-04-1.937634343D-06

1.793372625D-09	-5.672295580D-13						1.723135679D+04	-2.573912886D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8971.108

8.217238140D+05-2.850509348D+03 8.017266020D+00-2.105663212D-03 6.849136340D-07

-9.989129320D-11	5.192456840D-15						3.229372870D+04	-2.326810811D+01
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BeBr2 Gurvich,1996a pt1 p377 pt2 p302.

2 tpis96 BE	1.00BR	2.00	0.00	0.00	0.00	0	168.8201820	-234062.499
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12837.501

-2.118698678D+04 2.090382611D+02 3.731171310D+00 1.115501549D-02-1.542821761D-05

1.052354444D-08	-2.850006057D-12						-3.090456277D+04	9.458917720D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12837.501

-1.041331811D+05-1.543443092D+02 7.614465410D+00-4.556700630D-05 1.003180548D-08

-1.146879501D-12	5.301795380D-17						-2.984527608D+04	-1.149360980D+01
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BeCL Gurvich,1996a pt1 p369, pt2 p295.

2 tpis96 BE	1.00CL	1.00	0.00	0.00	0.00	0	44.4651820	56693.107
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8861.107

2.016138947D+04-1.413988978D+02 2.898223773D+00 6.069925510D-03-9.162038470D-06

6.612620660D-09	-1.859126853D-12						6.626691440D+03	7.900181050D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8861.107

2.808845146D+05-1.103100122D+03 5.671189830D+00-5.443000450D-04 1.459036606D-07

-1.230971735D-11	9.900804760D-17						1.224649804D+04	-8.382371370D+00
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BeCL2 Gurvich,1996a pt1 p373 pt2 p298.

2 tpis96 BE	1.00CL	2.00	0.00	0.00	0.00	0	79.9181820	-361539.140
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12080.860

-2.229957657D+04 1.528781667D+02 3.714994710D+00 1.067776550D-02-1.397766942D-05

9.066693560D-09	-2.350292311D-12						-4.590428230D+04	6.682555572D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12080.860

-1.154087460D+05-2.484300053D+02 7.685672140D+00-7.444960370D-05 1.649479787D-08

-1.895997075D-12	8.804973950D-17						-4.468747280D+04	-1.500337407D+01
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## Appendix D (continued)

BeF Gurvich,1996a pt1 p363, pt2 p291.

2 tpis96 BE	1.00F	1.00	0.00	0.00	0.00	0.00	0.00	28.0105852	-170624.795
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.664497230D+04	7.887178850D+02	-1.463363201D+00	1.381790494D-02	-1.591299964D-05					
9.352931520D-09	-2.229211181D-12			-2.522627476D+04	3.197634300D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.857941543D+05	4.776082770D+01	4.269986020D+00	2.310668473D-04	-6.657214920D-08					
1.152149888D-11	-6.335586440D-16			-2.257950960D+04	-2.184787270D-01				

BeF2 Gurvich,1996a pt1 p366 pt2 p293.

2 tpis96 BE	1.00F	2.00	0.00	0.00	0.00	0.00	0.00	47.0089884	-796588.236
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.490270240D+03	-2.878053102D+02	5.434712820D+00	3.903233460D-03	-2.214865601D-06					
-1.965806119D-10	4.042362270D-13			-9.591615640D+04	-5.616616920D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.482018070D+04	-7.684556060D+02	8.062860840D+00	-2.227502549D-04	4.891598660D-08					
-5.587886720D-12	2.583409761D-16			-9.395495490D+04	-2.125660266D+01				

BeH Gurvich,1996a pt1 p356, pt2 p286.

2 tpis96 BE	1.00H	1.00	0.00	0.00	0.00	0.00	0.00	10.0201220	342252.104
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.615149125D+03	-5.935286080D+01	4.507269100D+00	-5.264189610D-03	1.145319967D-05					
-9.247883590D-09	2.700364753D-12			4.030193040D+04	-3.485117050D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.424081636D+06	6.597398460D+03	-3.626316480D+00	4.579634350D-03	-1.163329056D-06					
1.297785691D-10	-5.291885810D-15			-2.489846221D+03	5.216018690D+01				

BeH+ Chase,1998 p391 9/66.

3 g 1/01 BE	1.00H	1.00E	-1.00	0.00	0.00	0.00	0.00	10.0195734	1178218.951
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.220611020D+04	2.520229596D+02	3.207719570D+00	-2.191287290D-03	6.902534490D-06					
-5.769522630D-09	1.656414969D-12			1.392530660D+05	3.307044770D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.622341590D+05	-1.760169629D+03	5.379905550D+00	2.742462444D-05	-1.167208170D-07					
3.557177910D-11	-2.569695765D-15			1.515859734D+05	-1.369222641D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.282300776D+08	-1.214880850D+05	2.642762928D+01	-1.410369386D-03	3.776812140D-08					
6.975949060D-14	-1.287263021D-17			1.127119075D+06	-2.060147218D+02				

BeH2 Martin,1992. Martin,1997.

2 g 4/01 BE	1.00H	2.00	0.00	0.00	0.00	0.00	0.00	11.0280620	161098.903
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.065314900D+04	-1.320657220D+03	9.901308060D+00	-1.255772231D-02	2.205704068D-05					
-1.633609388D-08	4.505103240D-12			2.464561869D+04	-3.635826750D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.074262010D+05	-3.407534250D+03	9.792370360D+00	-8.254614820D-04	1.915656246D-07					
-1.962774813D-11	8.929908660D-16			3.793105200D+04	-4.254653580D+01				

BeI Gurvich,1996a pt1 p378, pt2 p303.

2 tpis96 BE	1.00I	1.00	0.00	0.00	0.00	0.00	0.00	135.9166520	207454.309
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.530054810D+04	-5.190950260D+02	5.714505240D+00	-1.409073640D-03	7.664772120D-07					
-2.601945105D-11	-8.230960640D-14			2.637903657D+04	-5.140997840D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.328206620D+05	1.139497861D+03	3.629171660D+00	1.704033769D-04	1.067048688D-07					
-3.589457880D-11	2.722769560D-15			1.585474307D+04	9.370951270D+00				

BeI2 Gurvich,1996a pt1 p380 pt2 p305.

2 tpis96 BE	1.00I	2.00	0.00	0.00	0.00	0.00	0.00	262.8211220	-64759.451
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.592726180D+02	-4.866059010D+01	5.241571180D+00	7.830305060D-03	-1.169525374D-05					
8.389583910D-09	-2.356636003D-12			-9.333220920D+03	2.896318281D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.392372840D+04	-8.959214380D+01	7.565554790D+00	-2.577727326D-05	5.614265330D-09					
-6.359663850D-13	2.917080336D-17			-9.814768620D+03	-9.032042810D+00				

BeN Chase,1998 p403.

2 j 6/63 BE	1.00N	1.00	0.00	0.00	0.00	0.00	0.00	23.0188820	427000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.247783630D+04	7.590188900D+02	-1.561469235D+00	1.496945721D-02	-1.835608880D-05					
1.146861461D-08	-2.897470581D-12			4.683003320D+04	3.256973759D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.909696160D+04	-3.078649431D+02	4.727959150D+00	-3.928158830D-05	2.006201069D-08					
-2.300018068D-12	1.066101831D-16			5.156095710D+04	-3.031380625D+00				

## Appendix D (continued)

BeO Gurvich,1996a pt1 p351, pt2 p280.

3 tps96 BE	1.000	1.00	0.00	0.00	0.00	0	25.0115820	128940.304
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8688.104
-4.869458320D+04	7.213473620D+02	-3.784157320D-01	8.792203850D-03	-7.070151260D-06				
2.250175620D-09	-2.799117872D-14		1.101466639D+04	2.574081184D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8688.104
-3.503472450D+07	1.055859473D+05	-1.165011722D+02	6.477369480D-02	-1.649656058D-05				
2.005558400D-09	-9.426891790D-14		-6.570018000D+05	8.640898030D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8688.104
-7.440106320D+07	4.309665300D+04	-1.019586064D-01	2.617209088D-04	-2.461810861D-08				
1.124733698D-12	-1.832802285D-17		-3.402379380D+05	4.487040230D+01				

BeOH Gurvich,1996a pt1 p358 pt2 p288.

2 tps96 BE	1.000	1.00H	1.00	0.00	0.00	0	26.0195220	-99717.721
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10798.450
-3.853024520D+04	4.498059290D+02	1.532096459D+00	1.299912603D-02	-1.708979996D-05				
1.169968182D-09	-3.163183710D-12		-1.559046567D+04	1.545542930D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10798.450
8.550330310D+05	-2.646537838D+03	8.204784630D+00	1.110814513D-05	-4.265364000D-08				
7.926511920D-12	-4.645419520D-16		3.121216271D+03	-2.571641308D+01				

BeOH+ Chase,1998 p393.

3 j12/75 BE	1.000	1.00H	1.00E	-1.00	0.00	0	26.0189734	759983.920
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9550.904
7.106119160D+04	-8.068981600D+02	5.603107810D+00	4.932070860D-03	-7.722847160D-06				
5.910889810D-09	-1.695201901D-12		9.440782420D+04	-1.088099852D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9550.904
8.134874390D+05	-2.814653683D+03	8.381145010D+00	-6.942073280D-05	-2.369535806D-08				
5.678106380D-12	-3.583253560D-16		1.073129932D+05	-2.901093335D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9550.904
-6.279111750D+06	2.090044240D+03	7.025559910D+00	5.492111300D-05	-3.446137200D-09				
1.115947764D-13	-1.461494242D-18		6.914837000D+04	-1.732443156D+01				

Be(OH)2 Gurvich,1996a pt1 p360 pt2 p290.

2 tps96 BE	1.000	2.00H	2.00	0.00	0.00	0	43.0268620	-638864.416
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15225.858
7.863089830D+03	-7.397142250D+02	1.043303334D+01	4.514249530D-03	-6.950601530D-06				
5.777030040D-09	-1.727199382D-12		-7.585676960D+04	-3.301466610D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15225.858
1.722889403D+06	-5.242477190D+03	1.486877785D+01	3.931498360D-05	-8.920276310D-08				
1.630912925D-11	-9.505371140D-16		-4.642823840D+04	-6.476804020D+01				

BeS Gurvich,1996a pt1 p381 pt2 p307.

2 tps96 BE	1.00S	1.00	0.00	0.00	0.00	0	41.0771820	247095.306
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8780.106
-7.390579080D+03	2.828134792D+02	6.552019400D-01	1.076012495D-02	-1.398380157D-05				
8.818418890D-09	-2.110588578D-12		2.751593294D+04	1.980493561D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8780.106
-1.655708361D+07	5.431466120D+04	-6.351859250D+01	3.964091990D-02	-1.078978696D-05				
1.394030343D-09	-6.936955040D-14		-3.121559628D+05	4.803454935D+02				

Be2 Gurvich,1996a pt1 p346 pt2 p277.

2 tps96 BE	2.00	0.00	0.00	0.00	0.00	0	18.0243640	637543.318
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9838.118
-1.580873810D+05	2.035567774D+03	-3.691580630D+00	1.028818435D-02	-9.603854510D-06				
4.707519420D-09	-9.374688790D-13		6.526968370D+04	4.879324990D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9838.118
1.010034484D+05	1.414207488D+02	2.292070182D+00	1.543331824D-04	-5.801043000D-08				
1.003129697D-11	-5.682818340D-16		7.550139730D+04	1.238758616D+01				

Be2CL4 Gurvich,1996a pt1 p374 pt2 p299.

2 tps96 BE	2.00CL	4.00	0.00	0.00	0.00	0	159.8363640	-819604.973
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								22641.384
1.216152589D+05	-2.000824823D+03	1.723384275D+01	5.810448280D-03	-1.362970089D-05				
1.156602362D-08	-3.552255800D-12		-9.206475470D+04	-6.137959774D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								22641.384
-3.354920080D+05	-2.316199283D+02	1.617047912D+01	-6.734405950D-05	1.472073032D-08				
-1.672352806D-12	7.688773970D-17		-1.031075197D+05	-5.047009374D+01				

Be2F4 Gurvich,1996a pt1 p368 pt2 p294.

2 tps96 BE	2.00F	4.00	0.00	0.00	0.00	0	94.0179768	-1731699.842
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								19834.508
-6.327701870D+03	-6.902533720D+01	5.470937230D+00	3.097341347D-02	-4.094310060D-05				
2.668113685D-08	-6.942909560D-12		-2.105979269D+05	-2.073546195D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								19834.508
-3.681834950D+05	-9.439191480D+02	1.670099855D+01	-2.797974015D-04	6.178061720D-08				
-7.083080190D-12	3.282791040D-16		-2.089045725D+05	-6.092665760D+01				

## Appendix D (continued)

Be20 Gurvich,1996a pt1 p353 pt2 p282.

2 tpis96 BE	2.000	1.00	0.00	0.00	0.00	0.00	0	34.0237640	-37033.803
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.263673570D+02	-1.159556261D+02	4.082677770D+00	1.015885064D-02	-1.326015538D-05					
8.488955360D-09	-2.168039077D-12		-5.362258120D+03	1.253737886D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.412646378D+05	-3.498644590D+02	7.760932680D+00	-1.044953518D-04	2.313342334D-08					
-2.657722263D-12	1.233820439D-16		-5.172385490D+03	-1.854887619D+01					

Be20F2 Chase,1998 p417.

2 j 6/66 BE	2.000	1.00F	2.00	0.00	0.00	0	72.0205704	-1204574.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.783491921D+04	1.782881461D+02	4.094251360D+00	2.270142496D-02	-2.672688189D-05					
1.572575618D-08	-3.736070580D-12		-1.480081903D+05	7.353494770D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.281826506D+05	-1.130355396D+03	1.383400563D+01	-3.316080640D-04	7.304921010D-08					
-8.362704380D-12	3.872184980D-16		-1.431390587D+05	-4.739150230D+01					

Be202 Gurvich,1996a pt1 p354 pt2 p283.

2 tpis96 BE	2.000	2.00	0.00	0.00	0.00	0	50.0231640	-411635.309	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.031719530D+04	1.163353177D+03	-8.733155950D+00	5.372002930D-02	-7.279439190D-05					
4.894928250D-08	-1.312147056D-11		-5.546936880D+04	6.953282640D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.960576640D+05	-9.074948830D+02	1.067160422D+01	-2.670905218D-04	5.877629990D-08					
-6.718664090D-12	3.105949075D-16		-4.861114330D+04	-3.616546890D+01					

Be303 Gurvich,1996a pt1 p355 pt2 p284.

2 tpis96 BE	3.000	3.00	0.00	0.00	0.00	0	75.0347460	-1023720.628	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.738072346D+04	8.743832600D+02	-6.599606120D+00	6.533021140D-02	-8.762305740D-05					
5.817244790D-08	-1.540600500D-11		-1.284679012D+05	5.837203120D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.890809360D+05	-1.392823588D+03	1.703450699D+01	-4.127330740D-04	9.107529150D-08					
-1.043465231D-11	4.833053770D-16		-1.219045534D+05	-7.000614510D+01					

Be404 Gurvich,1996a pt1 p356 pt2 p285.

2 tpis96 BE	4.000	4.00	0.00	0.00	0.00	0	100.0463280	-1649294.582	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.893255640D+04	1.687565069D+03	-1.479616594D+01	1.007319774D-01	-1.291057622D-04					
8.243136760D-08	-2.111283987D-11		-2.072877151D+05	1.002507262D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.841338460D+05	-2.726394165D+03	2.402941774D+01	-8.114675460D-04	1.794255972D-07					
-2.059359498D-11	9.552905330D-16		-1.923710587D+05	-1.136620750D+02					

Br Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.

3 g 3/97 BR	1.00	0.00	0.00	0.00	0.00	0	79.9040000	111870.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.700293910D+03	6.145215420D+01	2.092120721D+00	1.376818870D-03	-2.445566658D-06					
2.050975161D-09	-5.144249091D-13		1.242508647D+04	8.996166200D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.789717400D+06	1.692051999D+04	-2.024085357D+01	1.395620355D-02	-3.656230560D-06					
4.489781000D-10	-2.122507526D-14		-9.207054960D+04	1.661695929D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.240248003D+08	7.034034730D+04	-1.023087313D+01	1.373755814D-03	-7.476473480D-08					
2.160883187D-12	-2.659054603D-17		-5.563101070D+05	1.226657143D+02					

Br+ Moore,1971. Moore,1970a. Gordon,1999.

3 g10/97 BR	1.00E	-1.00	0.00	0.00	0.00	0	79.9034514	1257927.034	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.981187420D+04	-4.751581470D+02	4.734578980D+00	-5.169324790D-03	5.905857520D-06					
-2.885129283D-09	5.054894290D-13		1.529052046D+05	-5.769283220D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.741149829D+06	-5.455465670D+03	8.470663350D+00	-2.683465574D-03	6.590454560D-07					
-7.953770300D-11	3.735898818D-15		1.851781643D+05	-3.637909030D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.174903280D+07	3.641704160D+04	-5.739744680D+00	1.067497350D-03	-7.127689890D-08					
2.155618820D-12	-1.769476126D-17		-1.399767498D+05	7.931577700D+01					



## Appendix D (continued)

Br- Hotop,1985. Gordon,1999.

3	g10/97 BR	1.00E	1.00	0.00	0.00	0.00	0	79.9045486	-219000.472	
	298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00						-2.708492743D+04	5.419556170D+00	
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00						-2.708492743D+04	5.419556170D+00	
	6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00						-2.708492743D+04	5.419556170D+00	

BrCL Gurvich,1989 pt1 p213 pt2 p112.

2	tpis89 BR	1.00CL	1.00	0.00	0.00	0.00	0	115.3570000	14789.113	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	1.653291583D+04	-3.578769280D+02	5.700622160D+00	-2.201257188D-03	2.415146969D-06					
	-1.371032976D+09	3.227803420D-13			2.252619279D+03	-4.155659669D+00				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-1.284863067D+05	-1.138379626D+03	7.964040800D+00	-3.438056670D-03	1.524999514D-06					
	-2.761469114D-10	1.694450407D-14			5.938264260D+03	-1.925044389D+01				

BrF Gurvich,1989 pt1 p208 pt2 p109.

2	tpis89 BR	1.00F	1.00	0.00	0.00	0.00	0	98.9024032	-58851.445	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	3.836143190D+04	-5.184611970D+02	5.458327050D+00	-5.656843100D-04	-4.121311970D-07					
	7.859913480D-10	-3.036161520D-13			-5.595539910D+03	-4.901129500D+00				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	3.771388470D+06	-1.267493430D+04	2.080555930D+01	-1.026359360D-02	3.308203590D-06					
	-4.903192250D-10	2.648275080D-14			7.062609720D+04	-1.130253600D+02				

BrF3 Gurvich,1989 pt1 p211 pt2 p110.

2	tpis89 BR	1.00F	3.00	0.00	0.00	0.00	0	136.8992096	-255600.000	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	1.116455127D+05	-1.959424330D+03	1.526220126D+01	-7.999362300D-03	6.982030260D-06					
	-3.242757960D-09	6.164751460D-13			-2.345341551D+04	-5.522633600D+01				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-1.886532240D+05	-8.245232970D+01	1.006180694D+01	-2.477319092D-05	5.478576860D-09					
	-6.282655260D-13	2.910628214D-17			-3.386800370D+04	-2.298937369D+01				

BrF5 Gurvich,1989 pt1 p212 pt2 p111.

2	tpis89 BR	1.00F	5.00	0.00	0.00	0.00	0	174.8960160	-428800.000	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	2.211366805D+05	-4.024809220D+03	2.734900212D+01	-1.832254979D-02	1.721754649D-05					
	-8.753508630D-09	1.860196959D-12			-3.537447670D+04	-1.244296466D+02				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-3.757647640D+05	-1.575896472D+02	1.611869838D+01	-4.776497800D-05	1.059755365D-08					
	-1.218527723D-12	5.657535450D-17			-5.667266800D+04	-5.540839310D+01				

BrO Chase,1996a.

2	j 3/96 BR	1.000	1.00	0.00	0.00	0.00	0	95.9034000	125800.000	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	1.455431116D+04	1.225152439D+02	-3.058728672D-01	2.117309202D-02	-3.494261190D-05					
	2.622639719D-08	7.508059540D-12			1.389149932D+04	2.527867438D+01				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-2.392612795D+06	6.932793130D+03	-2.513183892D+00	3.446544560D-03	-7.569536840D-07					
	6.514291340D-11	-1.715768736D-15			-3.084499064D+04	5.361048360D+01				

OBrO Chase,1996a.

2	j 3/96 BR	1.000	2.00	0.00	0.00	0.00	0	111.9028000	151954.526	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	3.470213230D+04	-3.401341820D+02	3.932251620D+00	1.215938586D-02	-1.901501702D-05					
	1.398631495D-08	-3.992899760D-12			1.875955788D+04	6.361235180D+00				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-1.624504660D+05	-1.453689372D+02	7.105822130D+00	-4.141362070D-05	8.981833260D-09					
	-1.013712869D-12	4.635133140D-17			1.650075386D+04	-9.111817920D+00				

BrOO Chase,1996a.

2	j 3/96 BR	1.000	2.00	0.00	0.00	0.00	0	111.9028000	108000.000	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-4.417619900D+04	4.959637160D+02	3.239884950D+00	5.941502110D-03	-3.402696770D-06					
	-3.444778160D-11	4.811957950D-13			8.815221980D+03	1.607446878D+01				
	1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	6.172483480D+03	-6.585049660D+02	7.483955330D+00	-1.920530746D-04	4.226946170D-08					
	-4.837392610D-12	2.239741320D-16			1.460353470D+04	-9.850380240D+00				

## Appendix D (continued)

BrO3 Chase, 1996a.

2 j 3/96 BR	1.000	3.00	0.00	0.00	0.00	0.00	0.00	127.9022000	220820.685
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.063901881D+05	-1.501928813D+03	9.703657430D+00	8.133000760D-03	-1.531857845D-05					
1.199117619D-08	-3.512747870D-12		3.233135990D+04	-2.735125430D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									13100.841
-2.822851113D+05	-2.358973461D+02	1.017525279D+01	-6.978451050D-05	1.535701661D-08					
-1.754454950D-12	8.104100150D-17		2.401140140D+04	-2.588197197D+01					

Br2 Gurvich, 1989 pt1 p200 pt2 p104.

2 tpis89 BR	2.00	0.00	0.00	0.00	0.00	0.00	0.00	159.8080000	30910.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.497047540D+03	-2.350884557D+02	5.491934320D+00	-2.227573303D-03	2.932401703D-06					
-1.954889514D-09	5.312307890D-13		3.521475050D+03	-1.964151570D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									9725.117
-4.311698570D+06	1.111268634D+04	-5.555775610D+00	3.630516590D-03	-2.754164226D-07					
-6.217506760D-11	7.375341620D-15		-7.036584160D+04	7.878478020D+01					

BrBrO Chase, 1996a.

2 j 3/96 BR	2.000	1.00	0.00	0.00	0.00	0.00	0.00	175.8074000	168000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.617498037D+04	-2.464406776D+02	5.912858450D+00	4.980354280D-03	-8.099958250D-06					
6.072776260D-09	-1.753715313D-12		1.974012093D+04	2.009704963D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									13137.498
-8.537101750D+04	-6.487046070D+01	7.047159350D+00	-1.843088186D-05	3.992267860D-09					
-4.500687950D-13	2.055867395D-17		1.821566655D+04	-3.162186125D+00					

BrOBr Chase, 1996a.

2 j 3/96 BR	2.000	1.00	0.00	0.00	0.00	0.00	0.00	175.8074000	107639.006
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.405068910D+04	-1.062722566D+03	9.907866290D+00	-4.470492470D-03	3.913701070D-06					
-1.805444867D-09	3.366132550D-13		1.642921537D+04	-2.350319399D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									12399.058
-9.686660250D+04	-3.957395270D+01	7.029434380D+00	-1.171881908D-05	2.576958549D-09					
-2.941186078D-13	1.357198784D-17		1.076942321D+04	-5.697779380D+00					

C Hf: Douglas, 1955. Moore, 1970b. Gordon, 1999.

3 g 7/97 C	1.00	0.00	0.00	0.00	0.00	0.00	0.00	12.0107000	716680.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.495031470D+02	-9.649010860D-01	2.504675479D+00	-1.281448025D-05	1.980133654D-08					
-1.606144025D-11	5.314483411D-15		8.545763110D+04	4.747924288D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6535.895
-1.289136472D+05	1.719528572D+02	2.646044387D+00	-3.353068950D-04	1.742092740D-07					
-2.902817829D-11	1.642182385D-15		8.410597850D+04	4.130047418D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6535.895
4.432528010D+08	-2.886018412D+05	7.737108320D+01	-9.715281890D-03	6.649595330D-07					
-2.230078776D-11	2.899388702D-16		2.355273444D+06	-6.405123160D+02					

C+ Moore, 1970b. Gordon, 1999.

3 g 6/98 C	1.00E	-1.00	0.00	0.00	0.00	0.00	0.00	12.0101514	1809444.482
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.258535929D+03	-1.574575687D+00	2.503637730D+00	-5.202878370D-06	4.516908390D-09					
-2.181431053D-12	4.495047033D-16		2.168951913D+05	4.345699505D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6649.282
1.255112551D+04	-3.411874670D+01	2.543383218D+00	-2.805120849D-05	9.751641970D-09					
-1.736855394D-12	1.246191931D-16		2.171001786D+05	4.063913515D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6649.282
5.618135320D+05	-6.047058900D+03	5.884541470D+00	-7.211894530D-04	6.823484110D-08					
-2.599878590D-12	3.633868358D-17		2.581370458D+05	-2.280019759D+01					

C- Hotop, 1985. Gordon, 1999.

3 g 3/98 C	1.00E	1.00	0.00	0.00	0.00	0.00	0.00	12.0112486	588314.236
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.671291530D+00	-1.986169369D-03	2.500008638D+00	-1.976750928D-08	2.478947477D-11					
-1.610664044D-14	4.236506810D-18		7.001218550D+04	4.879570141D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6218.836
4.253175720D+00	5.778186480D-04	2.499999424D+00	2.836136231D-10	-7.327253420D-14					
9.478507810D-18	-4.830487320D-22		7.001217170D+04	4.879624211D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6218.836
1.223289007D+01	-5.196185830D-03	2.500001344D+00	-1.743497251D-10	1.206609009D-14					
-4.252419790D-19	5.992333270D-24		7.001221630D+04	4.879608421D+00					

## Appendix D (continued)

CBR Gurvich,1991 pt1 p157 pt2 p137.

2 tps91 C	1.00BR	1.00	0.00	0.00	0.00	0.00	0	91.9147000	490431.816
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.324446880D+03	-1.596366559D+02	4.857856590D+00	-4.389439160D-04	4.408863630D-07					
-2.281330618D-10	5.445618220D-14			5.847677250D+04	1.351169646D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.021862102D+06	-3.243484360D+03	8.388226560D+00	-2.242155508D-03	6.988355370D-07					
-9.719134370D-11	4.716976240D-15			7.805924060D+04	-2.518386915D+01				

CBR2 Gurvich,1991 pt1 p159 pt2 p138.

2 tps91 C	1.00BR	2.00	0.00	0.00	0.00	0	171.8187000	336623.319	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.248197840D+04	-1.128261230D+03	9.822303380D+00	-3.872748100D-03	2.904819596D-06					
-1.061380159D-09	1.297474642D-13			4.437771600D+04	-2.361121795D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.441431410D+05	4.215427830D+02	8.796797740D+00	-2.726562507D-03	1.336438546D-06					
-2.304854483D-13	4.494245593D-14			3.364618140D+04	-1.599565135D+01				

CBR3 Gurvich,1991 pt1 p160 pt2 p139.

2 tps91 C	1.00BR	3.00	0.00	0.00	0.00	0	251.7227000	235000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.563516260D+04	-1.275764123D+03	1.117190031D+01	2.341705749D-03	-6.540671410D-06					
5.736717140D-09	-1.777823046D-12			3.243215890D+04	-2.766468801D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.926498949D+05	-1.324072178D+02	1.009808665D+01	-3.895040820D-05	8.550445010D-09					
-9.747493680D-13	4.494245593D-17			2.541576129D+04	-1.866868947D+01				

CBR4 Kudchadker,1975.

2 g 8/99 C	1.00BR	4.00	0.00	0.00	0.00	0	331.6267000	79500.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.023083739D+05	-1.735600709D+03	1.651317914D+01	-3.147664747D-03	2.924135486D-07					
1.360605681D-09	-6.431758650D-13			1.500502543D+04	-5.536476760D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.059785072D+05	-1.048517002D+02	1.307772550D+01	-3.086857556D-05	6.775309810D-09					
-7.721837540D-13	3.559218240D-17			5.615893940D+03	-3.283787630D+01				

CCL Hf:Kumaran,1997. Gurvich,1991 pt1 p106 pt2 p81.

2 g 8/99 C	1.00CL	1.00	0.00	0.00	0.00	0	47.4637000	432611.058	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.707070049D+05	-1.463803497D+01	2.334108251D+00	7.202099130D-03	-1.034120045D-05					
7.228106700D-09	-1.985123755D-12			5.123350300D+04	1.200820386D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.900507630D+05	-2.075311460D+03	6.880017230D+00	-1.294796228D-03	3.883137980D-07					
-5.006981630D-11	2.218229619D-15			6.358922050D+04	-1.610664472D+01				

CCLBr3 Gurvich,1991 pt1 p171 pt2 p152.

2 tps91 C	1.00CL	1.00BR	3.00	0.00	0.00	0	287.1757000	65000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.021596752D+05	-1.746281176D+03	1.598215634D+01	-1.350975234D-03	-2.330039129D-06					
3.201856270D-09	-1.150412393D-12			1.341967771D+04	-5.285079043D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.282709343D+05	-1.277037936D+02	1.309470658D+01	-3.763326710D-05	8.264715600D-09					
-9.424237560D-13	4.345940760D-17			3.930463310D+03	-3.315414033D+01				

CCL2 Hf:Kumaran,1997. Jacox,1994. Shin,1990.

2 g 8/99 C	1.00CL	2.00	0.00	0.00	0.00	0	82.9167000	222940.147	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.509623150D+04	-1.034728559D+03	8.061704540D+00	1.487134213D-03	-4.564817110D-06					
3.954885810D-09	-1.166197091D-12			3.052409293D+04	-1.739691692D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.437455170D+06	1.958413353D+04	-1.604038625D+01	1.238833906D-02	-3.013367274D-06					
3.473468920D-10	-1.553272793D-14			-9.961242160D+04	1.556949315D+02				

CCL2Br2 Gurvich,1991 pt1 p170 pt2 p151.

2 tps91 C	1.00CL	2.00BR	2.00	0.00	0.00	0	242.7247000	10000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.018495619D+05	-1.740854039D+03	1.521338304D+01	1.128256510D-03	-5.875405490D-06					
5.659886970D-09	-1.821576512D-12			6.918572190D+03	-5.015385819D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.553347012D+05	-1.598005477D+02	1.311860930D+01	-4.717443870D-05	1.036912808D-08					
-1.183321687D-12	5.460612690D-17			-2.588636980D+03	-3.461705319D+01				

## Appendix D (continued)

CCL3                    Hf:Hudgens,1991. TRC(12/93) tuv7270.

2 n12/93 C	1.00CL	3.00	0.00	0.00	0.00	0.00	0	118.3697000	71128.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.414471650D+04	-5.547969730D+02	6.845544390D+00	1.242006495D-02	-2.036896881D-05					
1.554979993D-08	-4.568940110D-12		9.388568820D+03	-7.143598465D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.427572540D+05	6.809020620D+02	9.047723620D+00	1.324277766D-04	6.301263040D-08					
-2.656639200D-11	2.105668053D-15		3.866216150D+02	-1.528745849D+01					

CCL3Br                    Gurvich,1991 pt1 p169 pt2 p150.

2 tps91 C	1.00CL	3.00BR	1.00	0.00	0.00	0	198.2737000	-43000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.049688463D+05	-1.793828482D+03	1.489250892D+01	2.397128310D-03	-7.789615470D-06				
7.016617110D-09	-2.196069746D-12		9.101349310D+02	-5.058348139D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.772324186D+05	-1.840310333D+02	1.313673812D+01	-5.443910010D-05	1.197658923D-08				
-1.367818632D-12	6.316164790D-17		-8.895857690D+03	-3.669528209D+01				

CCL4                    Gurvich,1991 pt1 p111 pt2 p84.

2 tps91 C	1.00CL	4.00	0.00	0.00	0.00	0	153.8227000	-95600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.093385626D+05	-1.861731846D+03	1.449632467D+01	3.949485160D-03	-1.010805379D-05				
8.645514170D-09	-2.642368852D-12		-4.948006230D+03	-5.180284750D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.043078255D+05	-2.168170491D+02	1.316132386D+01	-6.431124890D-05	1.416482497D-08				
-1.619343320D-12	7.483974350D-17		-1.512320070D+04	-3.996844300D+01				

CF                    Hf:TRC(6/88) w6950. Gurvich,1991 pt1 p74 pt2 p55.

2 tps91 C	1.00F	1.00	0.00	0.00	0.00	0	31.0091032	242300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.582786680D+04	7.972635890D+02	-1.364936319D+00	1.312359375D-02	-1.457012892D-05				
8.253276680D-09	-1.896351845D-12		2.438259620D+04	3.248065280D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.329807100D+05	-1.214340891D+02	4.452413620D+00	1.293786948D-04	-3.670550590D-08				
6.590212390D-12	-3.731261610D-16		2.815934108D+04	-6.640468730D-01				

CF+                    Chase,1998 p579 12/70.

2 g12/99 C	1.00F	1.00E	-1.00	0.00	0.00	0	31.0085546	1145564.099
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.975213200D+04	9.276863650D+02	-1.866581982D+00	1.384340912D-02	-1.513428860D-05				
8.518556340D-09	-1.959577655D-12		1.323519410D+05	3.412013190D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.053762780D+04	-3.390275090D+02	4.708373500D+00	-3.963148310D-05	2.497996218D-08				
-5.236790430D-12	5.313949130D-16		1.381337068D+05	-3.920514730D+00				

CFBr3                    Gurvich,1991 pt1 p166 pt2 p146.

2 tps91 C	1.00F	1.00BR	3.00	0.00	0.00	0	270.7211032	-120000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.149244280D+04	-9.364796640D+02	1.044260886D+01	1.205370047D-02	-1.876290291D-05				
1.344488618D-08	-3.730545760D-12		-1.243246293D+04	-2.363948551D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.729158956D+05	-3.328164650D+02	1.324822519D+01	-9.927077540D-05	2.193640054D-08				
-2.515424945D-12	1.165680878D-16		-1.730185479D+04	-3.626818430D+01				

CFCL                    Hf:Gurvich,1991 pt1 p135 pt2 p107. Jacox,1994.

2 g 9/99 C	1.00F	1.00CL	1.00	0.00	0.00	0	66.4621032	25845.774
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.541997945D+04	-8.274039810D+01	2.501701822D+00	1.390738086D-02	-1.895734700D-05				
1.261934581D-08	-3.333453820D-12		2.411755114D+03	1.331517094D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.681630077D+05	-2.328091539D+00	6.834633830D+00	1.565270633D-04	-5.967755160D-08				
9.820924460D-12	-5.058897210D-16		3.017669604D+02	-9.005085129D+00				

CFCLBr2                    Gurvich,1991 pt1 p175 pt2 p158.

2 tps91 C	1.00F	1.00CL	1.00BR	2.00	0.00	0	226.2701032	-175000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.898799740D+04	-1.050714861D+03	1.039349401D+01	1.273690622D-02	-1.999097478D-05				
1.438204230D-08	-4.000130350D-12		-1.837799602D+04	-2.417479131D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.960811596D+05	-3.531276200D+02	1.326346169D+01	-1.053860298D-04	2.329085080D-08				
-2.670979639D-12	1.237844667D-16		-2.387594306D+04	-3.684977271D+01				

## Appendix D (continued)

CFCL2                      Gurvich,1991 pt1 p138 pt2 p110.

2 tps91 C	1.00F	1.00CL	2.00	0.00	0.00	0	101.9151032	-105000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.611398792D+04	-3.353565900D+02	4.094673080D+00	1.960244711D-02	-2.762775193D-05				
1.880124302D-08	-5.047410300D-12		-1.251298871D+04	6.870882561D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.653118323D+05	-4.469724170D+02	1.033334881D+01	-1.333673368D-04	2.948755634D-08				
-3.383306200D-12	1.568746348D-16		-1.393160489D+04	-2.556817972D+01				

CFCL2Br                      Gurvich,1991 pt1 p175 pt2 p157.

2 tps91 C	1.00F	1.00CL	2.00BR	1.00	0.00	0	181.8191032	-235000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.529959220D+04	-1.135235485D+03	1.009526872D+01	1.401380147D-02	-2.191705096D-05				
1.573404132D-08	-4.369340340D-12		-2.504488145D+04	-2.451093103D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.215455050D+05	-3.884129620D+02	1.328990796D+01	-1.160048581D-04	2.564498787D-08				
-2.941639768D-12	1.363542881D-16		-3.097421144D+04	-3.871356695D+01				

CFCL3                      Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p140 pt2 p112.

2 g 7/99 C	1.00F	1.00CL	3.00	0.00	0.00	0	137.3681032	-283700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.400174000D+04	-1.252282466D+03	1.001327229D+01	1.475107601D-02	-2.315635251D-05				
1.664207025D-08	-4.622929960D-12		-3.020508601D+04	-2.708387087D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.450464780D+05	-4.177821450D+02	1.331196736D+01	-1.248759531D-04	2.761391353D-08				
-3.168207640D-12	1.468834601D-16		-3.674067190D+04	-4.156886057D+01				

CF2                      Hf:TRC(6/88) w6950. Jacox,1998.

2 g 9/99 C	1.00F	2.00	0.00	0.00	0.00	0	50.0075064	-186600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.797026270D+04	8.731800030D+02	-3.460191570D+00	2.746253741D-02	-3.474621900D-05				
2.204470693D-08	-5.621750850D-12		-2.746797157D+04	4.456778070D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.086428547D+05	-5.854989140D+02	7.018648950D+00	3.929186150D-04	-2.603822675D-07				
-6.142196390D-11	-4.172833260D-15		-2.152945157D+04	-1.356143285D+01				

CF2+                      Chase,1998 p583 12/70. Jacox,1994.

2 g 9/99 C	1.00F	2.00E	-1.00	0.00	0.00	0	50.0069578	949341.299
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.892373827D+04	6.049354610D+02	-9.721866660D-01	1.808478341D-02	-1.980065782D-05				
1.101640055D-08	-2.500457119D-12		1.102755670D+05	3.247591470D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.488966070D+04	-1.064283593D+03	7.785702100D+00	-3.158347626D-04	7.130804080D-08				
-8.533183590D-12	4.251638820D-16		1.178446465D+05	-1.819424707D+01				

CF2Br2                      Gurvich,1991 pt1 p166 pt2 p145.

2 tps91 C	1.00F	2.00BR	2.00	0.00	0.00	0	209.8155064	-380000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.261404028D+04	-2.815725114D+02	5.098032130D+00	2.502548939D-02	-3.438853190D-05				
2.297615553D-08	-6.080161430D-12		-4.642763750D+04	3.094167118D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.327669300D+05	-6.184352490D+02	1.346170049D+01	-1.849172548D-04	4.092591340D-08				
-4.699810430D-12	2.180811799D-16		-4.715186610D+04	-4.105369240D+01				

CF2CL                      Gurvich,1991 pt1 p136 pt2 p108.

2 tps91 C	1.00F	2.00CL	1.00	0.00	0.00	0	85.4605064	-275000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.914558350D+03	-1.768816959D+01	1.607015025D+00	2.473626554D-02	-3.270738940D-05				
2.126351830D-08	-5.509831110D-12		-3.427306250D+04	1.929680690D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.802346654D+05	-6.860314850D+02	1.051143635D+01	-2.046954963D-04	4.528897180D-08				
-5.200229030D-12	2.412971450D-16		-3.308179480D+04	-2.874899785D+01				

CF2CLBr                      Gurvich,1991 pt1 p173 pt2 p156.

2 tps91 C	1.00F	2.00CL	1.00BR	1.00	0.00	0	165.3645064	-435000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.696699365D+04	-4.678832270D+02	5.244809420D+00	2.530121349D-02	-3.508443520D-05				
2.354353958D-08	-6.246161130D-12		-5.198382730D+04	8.532887803D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.592828840D+05	-6.539283590D+02	1.348831524D+01	-1.956099469D-04	4.329775970D-08				
-4.972644370D-12	2.307575050D-16		-5.365141170D+04	-4.224913908D+01				

## Appendix D (continued)

CF2CL2 Hf:TRC(6/89) w7350. Gurvich, 1991 pt1 p139 pt2 p111.

2 g 7/99 C	1.00F	2.00CL	2.00	0.00	0.00	0.00	0	120.9135064	-490800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.841258750D+04	-6.139499820D+02	5.269667190D+00	2.574105783D-02	-3.587376480D-05					
2.411600130D-08	-6.402236900D-12		-5.784541330D+04	-1.957454856D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.827448550D+05	-6.933774800D+02	1.351791274D+01	-2.075114435D-04	4.594021610D-08					
-5.276874600D-12	2.449037044D-16		-6.021527770D+04	-4.479580046D+01					

CF3 Hf:TRC(6/88) w6950. Jacox, 1998.

2 g 8/99 C	1.00F	3.00	0.00	0.00	0.00	0.00	0	69.0059096	-467400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.978307106D+04	7.153678830D+02	-3.498185380D+00	3.595457990D-02	-4.507974430D-05					
2.821808450D-08	-7.098047020D-12		-6.059997030D+04	4.502592640D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.997305557D+05	-1.046989457D+03	1.077923191D+01	-3.116087076D-04	6.891351430D-08					
-7.911225640D-11	3.670593020D-16		-5.425304400D+04	-3.417038790D+01					

CF3+ Chase, 1998 p583 12/71. Jacox, 1998.

2 g 9/99 C	1.00F	3.00E	-1.00	0.00	0.00	0.00	0	69.0053610	423617.480
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.587463540D+04	3.743506700D+02	7.787413930D-01	1.929435768D-02	-1.892815770D-05					
9.363908760D-09	-1.885759656D-12		4.775581720D+04	2.224044005D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.910919531D+04	-1.996658183D+03	1.144279678D+01	-5.653393040D-04	1.232297113D-07					
-1.399758046D-11	6.443017950D-16		5.902345800D+04	-4.080349990D+01					

CF3Br Gurvich, 1991 pt1 p165 pt2 p144.

2 tpis91 C	1.00F	3.00BR	1.00	0.00	0.00	0.00	0	148.9099096	-648800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.439489010D+03	1.243615190D+02	9.231941950D-01	3.481044380D-02	-4.549645490D-05					
2.932836552D-08	-7.548000360D-12		-8.023396760D+04	2.232999096D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.834088510D+05	-9.719093300D+02	1.372477396D+01	-2.901710612D-04	6.421892200D-08					
-7.375688770D-12	3.423154250D-16		-7.765306310D+04	-4.913411939D+01					

CF3CL Hf:TRC(6/89) w7350. Gurvich, 1991 pt1 p137 pt2 p109.

2 g 7/99 C	1.00F	3.00CL	1.00	0.00	0.00	0.00	0	104.4589096	-704200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.499409978D+04	-1.365768572D+02	1.452912370D+00	3.404765070D-02	-4.473777640D-05					
2.888115112D-08	-7.434171330D-12		-8.547166640D+04	1.727327095D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.066042120D+05	-1.022626507D+03	1.376252628D+01	-3.052722979D-04	6.755966040D-08					
-7.759315250D-12	3.601192290D-16		-8.410559370D+04	-4.913411939D+01					

CF4 Hf:TRC(12/94) w6520. Gurvich, 1991 pt1 p79 pt2 p58.

2 g 7/99 C	1.00F	4.00	0.00	0.00	0.00	0.00	0	88.0043128	-933120.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.817458500D+03	1.163343483D+02	-1.288338636D+00	3.959566910D-02	-4.996244210D-05					
3.125339346D-08	-7.841700320D-12		-1.138502297D+05	2.938656548D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.164456780D+05	-1.414797167D+03	1.405124837D+01	-4.199093860D-04	9.278921610D-08					
-1.064575830D-11	4.937099680D-16		-1.094691149D+05	-5.487105000D+01					

CH Gurvich, 1979 pt1 p37 pt2 p39.

3 tpis79 C	1.00H	1.00	0.00	0.00	0.00	0.00	0	13.0186400	597370.604
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.220590133D+04	-3.405411530D+02	5.531452290D+00	-5.794964260D-03	7.969554880D-06					
-4.465911590D-09	9.596338320D-13		7.240783270D+04	-9.107673050D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.060763440D+06	-5.396206660D+03	7.856293850D+00	-7.965907450D-04	1.764308305D-07					
-1.976386267D-11	5.030429510D-16		1.062236592D+05	-3.154757439D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.068368690D+08	4.575450540D+05	-9.843975080D+01	1.235244098D-02	-8.485608570D-07					
3.040410624D-11	-4.400315170D-16		-3.595851590D+06	8.953477440D+02					

CH+ Gurvich, 1991 pt1 p38 pt2 p32.

3 tpis91 C	1.00H	1.00E	-1.00	0.00	0.00	0.00	0	13.0180914	1630571.004
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.019607105D+04	-4.618141310D+02	6.225641190D+00	-7.775711800D-03	1.094489485D-05					
-6.675487910D-09	1.565232409D-12		1.972491928D+05	-1.431512811D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.102094670D+06	1.828354883D+04	-1.312691402D+01	6.191717360D-03	-2.909421253D-07					
-1.134243575D-10	1.105962085D-14		7.541296040D+04	1.243984829D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.160070489D+08	1.436699396D+05	-1.108443407D+01	1.562285754D-04	4.928498470D-08					
-2.896872362D-12	4.982255990D-17		-1.013672855D+06	1.489353241D+02					

## Appendix D (continued)

CHBr3 Kudchadker, 1975.

2 g	8/99 C	1.00H	1.00BR	3.00	0.00	0.00	0.00	0.00	252.7306400	16740.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15906.601
4.346576860D+04	-4.999634420D+02	5.620222110D+00	2.079346321D-02	-2.921336328D-05						
2.066942448D-08	-5.781220910D-12						2.627830062D+03	1.247904015D+00		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15906.601
6.274234950D+05	-3.378711100D+03	1.487852612D+01	-5.932745270D-04	1.082421577D-07						
-1.061012665D-11	4.319152450D-16						1.877234659D+04	-5.311909650D+01		

CHCL Hf:TRC(12/93) w7270. Gurvich, 1991. Jacox, 1998.

2 g	9/99 C	1.00H	1.00CL	1.00	0.00	0.00	0.00	0.00	48.4716400	297100.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10200.443
-2.699912334D+05	4.351199730D+03	-2.275911813D+01	7.550621760D-02	-9.071997970D-05						
5.256971860D-08	-1.189769182D-11						1.416862680D+04	1.520980812D+02		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10200.443
-9.548061900D+05	2.174413794D+03	4.867645370D+00	8.321641860D-04	-1.536948638D-07						
1.529236537D-11	6.596159360D-16						1.880121810D+04	2.674761385D+00		

CHCLBr2 Gurvich, 1991 pt1 p173 pt2 p155.

2 tpis91 C	1.00H	1.00CL	1.00BR	2.00	0.00	0.00	0.00	0.00	208.2796400	10000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15291.236
3.815380250D+04	-4.084175110D+02	4.639244020D+00	2.325990646D-02	-3.222988860D-05						
2.254671151D-08	-6.256507740D-12						1.483809044D+03	6.175235281D+00		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15291.236
6.042865300D+05	-3.438241010D+03	1.494162631D+01	-6.228427970D-04	1.153724426D-07						
-1.147291377D-11	4.733482860D-16						1.822460958D+04	-5.407258924D+01		

CHCL2 TRC(12/93) tuv7270.

2 n12/93 C	1.00H	1.00CL	2.00	0.00	0.00	0.00	0.00	0.00	83.9246400	95800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12800.000
5.638556130D+04	-6.562455420D+02	6.068818020D+00	9.744122600D-03	-1.275310131D-05						
8.552386720D-09	-2.231582700D-12						1.330447798D+04	-4.533535456D+00		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12800.000
8.849393710D+05	-3.526969730D+03	1.186372153D+01	-5.002376120D-04	6.133860400D-08						
-1.185433405D-12	-1.234221421D-16						3.071136475D+04	-4.088905858D+01		

CHCL2Br Gurvich, 1991 pt1 p172 pt2 p154.

2 tpis91 C	1.00H	1.00CL	2.00BR	1.00	0.00	0.00	0.00	0.00	163.8286400	-45000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14729.895
3.294022650D+04	-3.275301170D+02	3.773235240D+00	2.536466143D-02	-3.472666990D-05						
2.404666618D-08	-6.621730930D-12						-5.425565080D+03	9.433412004D+00		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14729.895
5.924876440D+05	-3.509475610D+03	1.499349593D+01	-6.433062570D-04	1.198581809D-07						
-1.198476716D-11	4.969948070D-16						1.197251405D+04	-5.602687781D+01		

CHCL3 Gurvich, 1991 pt1 p127 pt2 p98.

2 g	7/99 C	1.00H	1.00CL	3.00	0.00	0.00	0.00	0.00	119.3776400	-102700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14305.494
3.395333290D+04	-3.047428785D+02	2.923672263D+00	2.830547858D-02	-3.712424690D-05						
2.551365915D-08	-6.987659550D-12						-1.235063157D+04	1.115556408D+01		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14305.494
6.136052740D+05	-3.715087170D+03	1.510777247D+01	2.362584336D-04	1.297140438D-07						
-1.267494791D-11	5.259022310D-16						6.203313450D+03	-5.992576539D+01		

CHF Hf:TRC(6/88) w695. Jacox, 1998.

2 g	8/99 C	1.00H	1.00F	1.00	0.00	0.00	0.00	0.00	32.0170432	108800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9981.216
-7.868585830D+04	1.300218466D+03	-3.947685250D+00	2.114995848D-02	-2.239962738D-05						
1.283155181D-08	-2.904778136D-12						5.824389720D+03	4.785453770D+01		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9981.216
3.994085420D+06	-7.962756200D+03	6.755595090D+00	4.949836570D-03	-2.101763812D-06						
3.348232950D-10	-1.886825050D-14						6.706134940D+04	-2.381240379D+01		

CHFB2 Gurvich, 1991 pt1 p168 pt2 p149.

2 tpis91 C	1.00H	1.00F	1.00BR	2.00	0.00	0.00	0.00	0.00	191.8250432	-175000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14359.556
-1.820197980D+04	4.362249670D+02	-3.733854170D-01	3.388631400D-02	-4.371298530D-05						
2.889569295D-08	-7.683915110D-12						-2.465611586D+04	3.320478790D+01		
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14359.556
5.935751630D+05	-3.742656580D+03	1.517184031D+01	-7.158039030D-04	1.360636972D-07						
-1.385897355D-11	5.844209110D-16						-2.347676027D+03	-5.765783430D+01		

## Appendix D (continued)

CHFCL Gurvich,1991 pt1 p147 pt2 p121.

2 tps91 C	1.00H	1.00F	1.00CL	1.00	0.00	0	67.4700432	-83144.704
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.113008510D+04	1.377872745D+03	-6.484617240D+00	3.890972490D-02	-4.800735220D-05				
3.073300019D-08	7.982853410D-12		-1.751793745D+04	6.373895867D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.622163580D+05	-3.809007980D+03	1.223880469D+01	-7.467182750D-04	1.434767850D-07				
-1.475406631D-11	6.273780680D-16		1.018987746D+04	-4.658365563D+01				

CHFCLBr Gurvich,1991 pt1 p176 pt2 p159.

2 tps91 C	1.00H	1.00F	1.00CL	1.00BR	1.00	0	147.3740432	-230000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.959240614D+04	4.901723270D+02	-1.259408503D+00	3.617708470D-02	-4.654244960D-05				
3.065240659D-08	8.123903600D-12		-3.139900705D+04	3.710450945D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.800117510D+05	-3.823337850D+03	1.522809062D+01	-7.373906310D-04	1.407097155D-07				
-1.438245319D-11	6.083867150D-16		-8.552249900D+03	-5.903677705D+01				

CHFCL2 Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p149 pt2 p124.

2 g 7/99 C	1.00H	1.00F	1.00CL	2.00	0.00	0	102.9230432	-284900.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.734959015D+04	4.924913200D+02	-1.854635884D+00	3.782786280D-02	-4.863343040D-05				
3.197197630D-08	8.459057990D-12		-3.788749270D+04	3.801530544D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.640113020D+05	-3.887083300D+03	1.527760246D+01	-7.576487420D-04	1.452498792D-07				
-1.490796515D-11	6.328998500D-16		-1.484736185D+04	-6.167535516D+01				

CHF2 TRC(6/88) tuv6950.

2 n 6/88 C	1.00H	1.00F	2.00	0.00	0.00	0	51.0154464	-238900.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.469690117D+05	2.553397313D+03	-1.302627630D+01	5.438128460D-02	-6.713418790D-05				
4.287651730D-08	-1.110824216D-11		-4.179372160D+04	9.939930250D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.526806550D+05	-3.696009170D+03	1.208610573D+01	-6.498588100D-04	1.120846220D-07				
-9.814147010D-12	3.349192390D-16		-9.437068420D+03	-4.704416200D+01				

CHF2Br Gurvich,1991 pt1 p168 pt2 p148.

2 tps91 C	1.00H	1.00F	2.00BR	1.00	0.00	0	130.9194464	-422000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.714510160D+04	1.422544046D+03	-6.684393650D+00	4.738389150D-02	-5.830588750D-05				
3.695720470D-08	-9.495485280D-12		-5.878500930D+04	6.608639090D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.767706840D+05	-4.177716080D+03	1.550150581D+01	-8.490147290D-04	1.657177491D-07				
-1.727828054D-11	7.435627230D-16		-2.966147348D+04	-6.349380140D+01				

CHF2CL Hf:TRC(6/89) w7350. Gurvich,1991 pt1 p148 pt2 p123.

2 g 7/99 C	1.00H	1.00F	2.00CL	1.00	0.00	0	86.4684464	-482800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.240579410D+04	1.365510973D+03	-7.153222080D+00	4.854987970D-02	-5.948781670D-05				
3.750966190D-08	-9.589524420D-12		-6.565932800D+04	6.657212230D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.629493730D+05	-4.298673050D+03	1.558191398D+01	-8.789278480D-04	1.720248689D-07				
-1.797910869D-11	7.753391700D-16		-3.634067160D+04	-6.611261480D+01				

CHF3 Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p97 pt2 p72.

2 g 8/99 C	1.00H	1.00F	3.00	0.00	0.00	0	70.0138496	-693300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.095132260D+05	2.042273879D+03	-1.166213079D+01	5.785807770D-02	-6.857135060D-05				
4.212118380D-08	-1.053196888D-11		-9.395470050D+04	8.935920650D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.685232020D+05	-4.728361700D+03	1.586728516D+01	-7.382348650D-04	1.970841706D-07				
-2.062115571D-11	8.970599640D-16		-5.923196370D+04	-7.161273220D+01				

CHI3 Kudchadker,1975.

2 g 8/99 C	1.00H	1.00I	3.00	0.00	0.00	0	393.7320500	210873.600
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.252923590D+04	-7.242166470D+02	8.018623340D+00	1.470995487D-02	-2.163843469D-05				
1.594571452D-08	-4.601437960D-12		2.678186915D+04	-8.605054840D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.294205430D+05	-3.184061570D+03	1.479622178D+01	-5.749555500D-04	1.062025541D-07				
-1.052804696D-11	4.329720020D-16		4.103609800D+04	-4.901357390D+01				



## Appendix D (continued)

CH2 D0 (H2C-H): Ruscic, 1999. Jacox, 1998.

2 g 4/02 C	1.00H	2.00	0.00	0.00	0.00	0.00	0.00	14.0265800	390364.517
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.218921730D+04	-2.877601815D+02	4.203583820D+00	3.455405960D-03	-6.746193340D-06					
7.654571640D-09	-2.870328419D-12	0.000000000D+00	4.733624710D+04	-2.143628603D+00					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.550418031D+06	-7.971625390D+03	1.228924487D+01	-1.699122922D-03	2.991728605D-07					
-2.767007492D-11	1.051341740D-15	0.000000000D+00	9.642216890D+04	-6.094739910D+01					

CH2Br2 Kudchadker, 1975.

2 g 8/99 C	1.00H	2.00BR	2.00	0.00	0.00	0.00	173.8345800	-14770.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
4.79738010D+03	3.613859240D+02	-1.819592338D+00	3.477048340D-02	-4.498546180D-05				
3.068623685D-08	-8.434846340D-12		-4.481497060D+03	3.827123590D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.528284441D+06	-6.673414950D+03	1.670213316D+01	-1.166351237D-03	2.122634493D-07				
-2.075472240D-11	8.428577700D-16		3.600706640D+04	-7.448065490D+01				

CH2CL Hf:TRC(12/93) w7270. Gurvich, 1991 pt1 p122. Jacox, 1998.

2 g12/99 C	1.00H	2.00CL	1.00	0.00	0.00	0.00	49.4795800	119200.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-3.188585630D+04	6.333163210D+02	-1.164065495D+00	2.160586080D-02	-2.545462163D-05				
1.693887757D-08	-4.660078600D-12		1.020142540D+04	3.230835289D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.662438334D+06	-6.441125720D+03	1.359753722D+01	-1.140536810D-03	2.087760159D-07				
-2.052347186D-11	8.375772270D-16		5.212906120D+04	-6.148586271D+01				

CH2CLBr Gurvich, 1991 pt1 p171 pt2 p153.

2 tpis91 C	1.00H	2.00CL	1.00BR	1.00	0.00	0.00	129.3835800	-45000.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-1.307948755D+04	6.455860380D+02	-3.577349910D+00	3.833687230D-02	-4.864252050D-05				
3.261622330D-08	-8.852877390D-12		-9.402272530D+03	4.748806758D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.525016309D+06	-6.823334160D+03	1.682769102D+01	-1.219735119D-03	2.244964495D-07				
-2.219063248D-11	9.104705130D-16		3.320239920D+04	-7.637571062D+01				

CH2CL2 Gurvich, 1991 pt1 p125 pt2 p97.

2 tpis91 C	1.00H	2.00CL	2.00	0.00	0.00	0.00	84.9325800	-95000.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-2.509841179D+04	6.687667380D+02	-5.094669210D+00	4.150049990D-02	-5.199772150D-05				
3.445944260D-08	-9.270292520D-12		-1.638978840D+04	5.396890320D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.529279337D+06	-6.976954760D+03	1.694154931D+01	-1.265053995D-03	2.344766734D-07				
-2.333227421D-11	9.632834730D-16		2.806318171D+04	-7.949453510D+01				

CH2F TRC(6/88) tuv6950.

2 n 6/88 C	1.00H	2.00F	1.00	0.00	0.00	0.00	33.0249832	-31800.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-8.569712530D+04	1.392226749D+03	-4.382052590D+00	2.645916948D-02	-2.848145663D-05				
1.732706028D-08	-4.442061440D-12		-1.169444586D+04	5.049499200D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
2.535399502D+06	-9.358439020D+03	1.700366206D+01	-3.062919929D-03	7.612869080D-07				
-9.664554980D-11	4.844768100D-15		5.228391310D+04	-8.707551570D+01				

CH2FBr Gurvich, 1991 pt1 p167 pt2 p147.

2 tpis91 C	1.00H	2.00F	1.00BR	1.00	0.00	0.00	112.9289832	-215000.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-9.256109530D+04	1.811985865D+03	-9.698346870D+00	5.035848670D-02	-6.070272680D-05				
3.878250800D-08	-1.012615992D-11		-3.537509620D+04	8.140396050D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.539975462D+06	-7.231551360D+03	1.714566439D+01	-1.350184394D-03	2.538022824D-07				
-2.558977386D-11	1.069310946D-15		1.509604224D+04	-8.062053710D+01				

CH2FCL Hf:TRC(6/89) w7350. Gurvich, 1991 pt1 p147 pt2 p122.

2 g 7/99 C	1.00H	2.00F	1.00CL	1.00	0.00	0.00	68.4779832	-265700.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
-1.071340332D+05	2.081328396D+03	-1.155723697D+01	5.441482110D-02	-6.518622740D-05				
4.133159880D-08	-1.071935103D-11		-4.264756210D+04	9.035923547D+01				
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
1.536120418D+06	-7.378939730D+03	1.725797178D+01	-1.395645457D-03	2.639247747D-07				
-2.675653563D-11	1.123582778D-15		9.813710460D+03	-8.313642553D+01				

## Appendix D (continued)

CH2F2                      Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p96 pt2 p71.

2 g 8/99 C	1.00H	2.00F	2.00	0.00	0.00	0	52.0233864	-452300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.819917500D+05	3.174427890D+03	-1.714256906D+01	6.411353830D-02	-7.313592120D-05				
4.426384160D-08	-1.103877216D-11		-7.027058950D+04	1.207331926D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.546609496D+06	-7.876883330D+03	1.768770469D+01	-1.581298721D-03	3.068917255D-07				
-3.183405460D-11	1.363827177D-15		-9.800135960D+03	-8.907420360D+01				

CH2I2                      Kudchadker,1975. Kudchadker,1976.

2 g 8/99 C	1.00H	2.00I	2.00	0.00	0.00	0	267.8355200	117570.400
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.738133757D+04	-8.972568040D+01	1.387869408D+00	2.733482611D-02	-3.619408770D-05				
2.539187610D-08	-7.145585160D-12		1.338767276D+04	2.241870165D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.512892716D+06	-6.442912400D+03	1.659026137D+01	-1.135551520D-03	2.073750250D-07				
-2.033902231D-11	8.282283700D-16		5.058219030D+04	-7.125235140D+01				

CH3                      D0(H3C-H): Ruscic,1999. Jacox,1998.

2 g 4/02 C	1.00H	3.00	0.00	0.00	0.00	0	15.0345200	146658.040
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.876188806D+04	5.093268660D+02	2.002143949D-01	1.363605829D-02	-1.433989346D-05				
1.013556725D-08	-3.027331936D-12	0.000000000D+00	1.408271825D+04	2.022772791D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.760802663D+06	-9.336531170D+03	1.487729606D+01	-1.439429774D-03	2.444477951D-07				
-2.224555778D-11	8.395065760D-16	0.000000000D+00	7.481809480D+04	-7.919682400D+01				

CH3Br                      Kudchadker,1975.

2 g 8/99 C	1.00H	3.00BR	1.00	0.00	0.00	0	94.9385200	-37740.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.115585770D+04	1.524705928D+03	-8.230445210D+00	4.239973210D-02	-4.946979890D-05				
3.194433340D-08	-8.531237080D-12		-1.251753591D+04	7.048127770D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.524874348D+06	-1.011876098D+04	1.865902163D+01	-1.797673690D-03	3.298520110D-07				
-3.250912030D-11	1.330179925D-15		5.540576390D+04	-9.778664460D+01				

CH3CL                      Gurvich,1991 pt1 p122 pt2 p95.

2 tpis91 C	1.00H	3.00CL	1.00	0.00	0.00	0	50.4875200	-81870.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.841971100D+04	1.983700841D+03	-1.084512305D+01	4.777980050D-02	-5.515516260D-05				
3.506176140D-08	-9.236103960D-12		-1.994689506D+04	8.399658331D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.522463305D+06	-1.030115447D+04	1.882725852D+01	-1.872291294D-03	3.473372860D-07				
-3.458887220D-11	1.428941079D-15		5.111417410D+04	-1.006571389D+02				

CH3F                      Hf:TRC(12/89) w6880. Gurvich,1991 pt1 p93 pt2 p69.

2 g 8/99 C	1.00H	3.00F	1.00	0.00	0.00	0	34.0329232	-237700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.029821878D+05	3.447331130D+03	-1.768994275D+01	5.945275800D-02	-6.469528250D-05				
3.859418040D-08	-9.626541530D-12		-4.577926220D+04	1.228382176D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.561903188D+06	-1.086052758D+04	1.929446920D+01	-2.070973131D-03	3.929124530D-07				
-3.994503420D-11	1.681447081D-15		3.563508510D+04	-1.061158456D+02				

CH3I                      Kudchadker,1975.

2 g 8/99 C	1.00H	3.00I	1.00	0.00	0.00	0	141.9389900	13765.360
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.516462740D+04	1.086208429D+03	-5.663176270D+00	3.683171710D-02	-4.321393500D-05				
2.833483666D-08	-7.684383690D-12		-4.303830650D+03	5.688562690D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.511915982D+06	-9.960289990D+03	1.856907132D+01	-1.768191331D-03	3.242206260D-07				
-3.192942010D-11	1.305407821D-15		6.066929950D+04	-9.590777040D+01				

CH2OH                      Hydroxymethyl Radical. Johnson,1996.

2 g11/00 C	1.00H	3.00O	1.00	0.00	0.00	0	31.0339200	-17800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.560076238D+05	2.685446279D+03	-1.342022420D+01	5.757139470D-02	-7.284449990D-05				
4.836648860D-08	-1.293492601D-11		-1.596820410D+04	9.963033700D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.250349506D+06	-8.173186060D+03	1.599639179D+01	-8.704133720D-04	6.069183950D-08				
4.408349460D-12	-5.702309500D-16		4.645313430D+04	-7.835158450D+01				

## Appendix D (continued)

CH<sub>2</sub>OH+                      Hydroxymethyl Cation. Johnson,1996.

2 g11/00 C	1.00H	3.00O	1.00E	-1.00	0.00	0	31.0333714	716400.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-1.077080841D+05	2.252082711D+03	-1.188167865D+01	4.602316960D-02	-4.879736880D-05				
2.876413471D-08	7.100226500D-12		7.484447770D+04	9.027928570D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
2.603333487D+06	-1.009953810D+04	1.730843898D+01	-6.946390320D-04	3.009715083D-08				
5.221485980D-12	-5.090183790D-16		1.465402426D+05	-9.223955280D+01				

CH<sub>3</sub>O                      Hf:Gurvich,1991 pt1 p67. Jacox,1998 p271.

2 g 7/00 C	1.00H	3.00O	1.00	0.00	0.00	0	31.0339200	13000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
8.657117660D+04	-6.631685250D+02	2.257455672D+00	2.266283789D-02	-2.970566403D-05				
2.199341353D-08	-6.588043380D-12		4.174102130D+03	8.174777900D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
2.101188243D+06	-8.841968800D+03	1.822645731D+01	-1.743485034D-03	3.340434270D-07				
-3.728814690D-11	1.473897771D-15		5.309582060D+04	-9.422500590D+01				

CH<sub>4</sub>                      Gurvich,1991 pt1 p44 pt2 p36.

2 g 8/99 C	1.00H	4.00	0.00	0.00	0.00	0	16.0424600	-74600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-1.766850998D+05	2.786181020D+03	-1.202577850D+01	3.917619290D-02	-3.619054430D-05				
2.026853043D-08	-4.976705490D-12		-2.331314360D+04	8.904322750D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
3.730042760D+06	-1.383501485D+04	2.049107091D+01	-1.961974759D-03	4.727313040D-07				
-3.728814690D-11	1.623737207D-15		7.532066910D+04	-1.219124889D+02				

CH<sub>3</sub>OH                      Hf:TRC(6/87) w5030. Chen,1977.

2 g 7/00 C	1.00H	4.00O	1.00	0.00	0.00	0	32.0418600	-200940.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-2.416642886D+05	4.032147190D+03	-2.046415436D+01	6.903698070D-02	-7.598932690D-05				
4.598208360D-08	-1.158706744D-11		-4.433261170D+04	1.400142190D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
3.411570760D+06	-1.345500201D+04	2.261407623D+01	-2.141029179D-03	3.730050540D-07				
-3.498846390D-11	1.366073444D-15		5.636081560D+04	-1.277814279D+02				

CH<sub>3</sub>OOH                      Methyl Hydroperoxide, CH<sub>3</sub>-O-O-H. Dorofeeva,2001.

2 srd 01 C	1.00H	4.00O	2.00	0.00	0.00	0	48.0412600	-139000.000
200.000	1000.000 7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-1.497974156D+05	2.656222273D+03	-1.377060625D+01	6.588673830D-02	-7.751801650D-05				
4.968800700D-08	-1.314367640D-11	0.000000000D+00	-3.058414201D+04	1.031696850D+02				
1000.000	6000.000 7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
3.060740610D+06	-1.282959627D+04	2.541021168D+01	-2.394481095D-03	4.443429910D-07				
-4.416659500D-11	1.819673372D-15	0.000000000D+00	5.837492360D+04	-1.387713096D+02				

CI                      Gurvich,1991 pt1 p176 pt2 p160.

2 tpis91 C	1.00I	1.00	0.00	0.00	0.00	0	138.9151700	570200.814
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
1.043011064D+05	1.715427168D+03	1.288874952D+01	-1.828504834D-02	2.135468356D-05				
-1.286980869D-08	3.167047660D-12		7.550784700D+04	-4.496811320D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-2.408229894D+05	3.447387040D+02	4.976968700D+00	-8.444815390D-04	5.061239720D-07				
-1.047700525D-10	6.740843140D-15		6.451342020D+04	1.090913159D+00				

CI<sub>2</sub>                      Gurvich,1991 pt1 p178 pt2 p161.

2 tpis91 C	1.00I	2.00	0.00	0.00	0.00	0	265.8196400	468393.633
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
6.028289810D+04	-1.043205435D+03	1.017465942D+01	-5.535671710D-03	5.630319010D-06				
-3.108249657D-09	7.202469560D-13		5.964896550D+04	-2.310319208D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-7.028655530D+05	3.082750393D+02	9.046427050D+00	-2.946736644D-03	1.424347233D-06				
-2.453183410D-10	1.425270291D-14		5.021134210D+04	-1.560349377D+01				

CI<sub>3</sub>                      Gurvich,1991 pt1 p178 pt2 p162.

2 g 9/99 C	1.00I	3.00	0.00	0.00	0.00	0	392.7241100	405983.951
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
8.596784250D+04	-1.347703793D+03	1.272103659D+01	-2.442876357D-03	2.511609978D-07				
1.024658583D-09	-4.872692960D-13		5.310716510D+04	-3.238492900D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-1.536511918D+05	-8.357044370D+01	1.006203125D+01	-2.466447336D-05	5.419054750D-09				
-6.181417000D-13	2.851262022D-17		4.582589530D+04	-1.494825345D+01				

## Appendix D (continued)

CI4 Kudchadker, 1975. Kudchadker, 1976.

2 g 8/99 C	1.00I	4.00	0.00	0.00	0.00	0.00	0	519.6285800	267943.360
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.919043870D+04	-1.651906475D+03	1.796124325D+01	-8.518114250D-03	8.508682250D-06					
-4.599097730D-09	1.039492403D-12		3.689392150D+04	-5.805953120D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.446762770D+05	-5.280365170D+01	1.303985589D+01	-1.606214814D-05	3.567550470D-09					
-4.105366980D-13	1.907272766D-17		2.817746618D+04	-2.810414436D+01					

CN Hf: Huang, 1992. Gurvich, 1979 pt1 p212 pt2 p210.

3 g 8/99 C	1.00N	1.00	0.00	0.00	0.00	0	26.0174000	438683.552	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.949148570D+03	-1.391590572D+02	4.930835320D+00	-6.304670510D-03	1.256836472D-05					
-9.878300500D-09	2.843137221D-12		5.228455380D+04	-2.763115585D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.228006270D+06	5.040733390D+03	-2.121897722D-01	1.354901134D-03	1.325929798D-07					
-6.937006370D-11	5.494952270D-15		1.784496132D+04	3.282563919D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.794798118D+08	1.054346069D+05	-1.729624170D+01	2.194895530D-03	-8.508938030D-08					
9.318692990D-13	6.358139930D-18		-7.962594120D+05	1.913139639D+02					

CN+ Gurvich, 1991 pt1 p215 pt2 p203.

3 tpis91 C	1.00N	1.00E	-1.00	0.00	0.00	0	26.0168514	1798890.904	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.302909570D+05	8.775687500D+03	-2.977443560D+01	4.976897060D-02	-1.302225951D-05					
-2.058325353D-08	1.126843895D-11		1.703860539D+05	2.039918818D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.153463080D+06	1.857250421D+04	-1.084534159D+01	6.106681430D-03	-1.191208566D-06					
1.184848778D-10	-4.799838730D-15		9.242644960D+04	1.135340573D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.354919695D+08	1.433776703D+05	-2.975360271D+01	4.280545600D-03	-2.707260413D-07					
8.178340660D-12	-9.629506200D-17		-9.229047140D+05	2.964624987D+02					

CN- Gurvich, 1991 pt1 p218 pt2 p205.

2 tpis91 C	1.00N	1.00E	1.00	0.00	0.00	0	26.0179486	63885.104	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.606541390D+04	4.294174750D+02	2.328781880D+00	-1.235303004D-04	4.478462770D-06					
-4.403151290D-09	1.349001191D-12		4.362078340D+03	1.142928617D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.517964720D+05	-1.630477359D+03	5.609875750D+00	-3.975605970D-04	8.856147080D-08					
-9.722872320D-12	4.434205690D-16		1.647976581D+04	-1.175502699D+01					

CNN Gurvich, 1991 pt1 p220 pt2 p208. Jacox, 1994.

2 g12/99 C	1.00N	2.00	0.00	0.00	0.00	0	40.0241000	633484.056	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.357692360D+04	9.652438660D+02	-1.704121157D+00	2.037239025D-02	-2.183423906D-05					
1.176082777D-08	-2.551355221D-12		7.021729830D+04	3.528150910D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.817148765D+05	-6.729863490D+02	7.857948340D+00	-6.136880720D-05	-1.088178985D-08					
4.456655810D-12	-2.836496278D-16		7.723488980D+04	-1.966012324D+01					

CO Gurvich, 1979 pt1 p25 pt2 p29.

3 tpis79 C	1.000	1.00	0.00	0.00	0.00	0	28.0101000	-110535.196	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.489045326D+04	-2.92285939D+02	5.724527170D+00	-8.176235030D-03	1.456903469D-05					
-1.087746302D-08	3.027941827D-12		-1.303131878D+04	-7.859241350D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.619197250D+05	-1.944704863D+03	5.916714180D+00	-5.664282830D-04	1.398814540D-07					
-1.787680361D-11	9.620935570D-16		-2.466261084D+03	-1.387413108D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.868662960D+08	-7.500377840D+05	2.495474979D+02	-3.956351100D-02	3.297772080D-06					
-1.318409933D-10	1.998937948D-15		5.701421130D+06	-2.060704786D+03					

CO+ Gurvich, 1991 pt1 p26 pt2 p22.

3 tpis91 C	1.000	1.00E	-1.00	0.00	0.00	0	28.0095514	1247789.204	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.178786658D+04	1.288857032D+02	3.769057550D+00	-3.431730130D-03	8.193945750D-06					
-6.463814690D-09	1.803727574D-12		1.482345898D+05	3.990547070D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.316847506D+05	-1.057646148D+03	4.554257780D+00	4.495520320D-04	-2.489507047D-07					
5.267566420D-11	-3.289510270D-15		1.555050724D+05	-3.873462640D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.035604054D+08	2.393118392D+05	-7.034999240D+01	1.139551440D-02	-8.315173100D-07					
2.863705515D-11	-3.803269410D-16		-1.688617704D+06	6.291980420D+02					

## Appendix D (continued)

COCL                   Gurvich,1991 pt1 p118 pt2 p91.

2 tps91 C	1.000	1.00CL	1.00	0.00	0.00	0	63.4631000	-16000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.513175740D+04	-5.969189670D+02	8.327671350D+00	-7.056132590D-03	1.313150734D-05				
-1.037059653D-08	3.033665179D-12		-7.052770320D+02	-1.580716775D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.443720240D+05	-1.793143470D+03	8.392755900D+00	-5.374769590D-04	9.113555710D-08				
-3.111441728D-12	-2.040435218D-16		6.914470150D+03	-1.998919104D+01				

COCL2                   Gurvich,1991 pt1 p119 pt2 p92.

2 tps91 C	1.000	1.00CL	2.00	0.00	0.00	0	98.9161000	-219500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.319321450D+04	-1.577971273D+03	1.208353907D+01	-4.809015610D-03	7.688477320D-06				
-5.858841200D-09	1.687786559D-12		-2.054252334D+04	-3.834767320D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.545881891D+04	-1.305958516D+03	1.092922584D+01	-3.601210160D-04	7.787017650D-08				
-8.792452030D-12	4.028696610D-16		-2.219847340D+04	-3.233303450D+01				

COFCL                   Gurvich,1991 pt1 p146 pt2 p120.

2 tps91 C	1.000	1.00F	1.00CL	1.00	0.00	0	82.4615032	-429492.862
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.262173900D+04	-1.019738175D+03	7.290911990D+00	7.420691710D-03	-7.902548080D-06				
4.209427650D-09	-9.314412900D-13		-4.804386460D+04	-1.316923671D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.316887910D+04	-1.581009678D+03	1.112696501D+01	-4.373000800D-04	9.464190710D-08				
-1.069291346D-11	4.901756640D-16		-4.599667230D+04	-3.525879824D+01				

COF2                   Gurvich,1991 pt1 p89 pt2 p66.

2 tps91 C	1.000	1.00F	2.00	0.00	0.00	0	66.0069064	-640000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.263393150D+04	-4.618603390D+02	2.774114516D+00	1.831931082D-02	-2.130172554D-05				
1.266924542D-08	-3.101675983D-12		-7.564255100D+04	9.467181460D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.073806850D+04	-1.974009812D+03	1.140363654D+01	-5.437111470D-04	1.175232744D-07				
-1.326564192D-11	6.076772130D-16		-6.907795410D+04	-4.009695000D+01				

COHCL                   Gurvich,1991 pt1 p134 pt2 p106.

2 tps91 C	1.000	1.00H	1.00CL	1.00	0.00	0	64.4710400	-164211.876
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.332946870D+03	8.120365590D+01	1.374648391D+00	1.650970564D-02	-1.692917241D-05				
9.684046830D-09	-2.374469390D-12		-2.120356580D+04	1.938379650D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.318952850D+05	-4.416870840D+03	1.270661114D+01	-9.361408630D-04	1.855335611D-07				
-1.958378539D-11	8.512046830D-16		4.330496440D+03	-5.145071542D+01				

COHF                   Gurvich,1991 pt1 p106 pt2 p80.

2 tps91 C	1.000	1.00H	1.00F	1.00	0.00	0	48.0164432	-374590.361
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.585828500D+04	-1.048202675D+03	-4.776574220D+00	3.080719931D-02	-3.415895900D-05				
2.034926806D-08	-5.054194620D-12		-5.085983730D+04	5.232247410D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.578853160D+05	-4.791959120D+03	1.293975218D+01	-1.018285299D-03	2.021278474D-07				
-2.136698091D-11	9.299588910D-16		-1.878933107D+04	-5.527449140D+01				

COS                   Gurvich,1991 pt1 p211 pt2 p200.

2 g 5/01 C	1.000	1.00S	1.00	0.00	0.00	0	60.0751000	-141700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.547876430D+04	-1.319464821D+03	9.735257240D+00	-6.870830960D-03	1.082331416D-05				
-7.705597340D-09	2.078570344D-12		-1.191657685D+04	-2.991988593D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.959098567D+05	-1.756167688D+03	8.710430340D+00	-4.139424960D-04	1.015243648D-07				
-1.159609663D-11	5.691053860D-16		-8.927096690D+03	-2.636328016D+01				

CO2                   Gurvich,1991 pt1 p27 pt2 p24.

3 g 9/99 C	1.000	2.00	0.00	0.00	0.00	0	44.0095000	-393510.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.943650540D+04	-6.264116010D+02	5.301725240D+00	2.503813816D-03	-2.127308728D-07				
-7.689988780D-10	2.849677801D-13		-4.528198460D+04	-7.048279440D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.176962419D+05	-1.788791477D+03	8.291523190D+00	-9.223156780D-05	4.863676880D-09				
-1.891053312D-12	6.330036590D-16		-3.908350590D+04	-2.652669281D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.544423287D+09	1.016847056D+06	-2.561405230D+02	3.369401080D-02	-2.181184337D-06				
6.991420840D-11	-8.842351500D-16		-8.043214510D+06	2.254177493D+03				

## Appendix D (continued)

CO2+ Gurvich,1991 pt1 p30 pt2 p26.

3 g 9/99 C	1.000	2.00E	-1.00	0.00	0.00	0.00	0.00	44.0089514	944687.989
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.383030980D+04	1.086211742D+03	-2.771112737D+00	2.318463595D-02	-2.570240315D-05					
1.450335497D-08	-3.334470420D-12		1.071784918D+05	4.054885210D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.695051682D+05	-8.066469730D+02	8.002828460D+00	-1.577214041D-04	2.566759314D-08					
-2.404195965D-12	1.677446800D-16		1.154389478D+05	-2.133567772D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.365409060D+07	5.333327510D+04	-5.621698360D+00	1.491439440D-03	-7.553254510D-08					
1.794658103D-12	-1.627521598D-17		-3.111917656D+05	9.673884890D+01					

COOH Gurvich,1991 pt1 p60 pt2 p46.

2 tpis91 C	1.000	2.00H	1.00	0.00	0.00	0.00	0.00	45.0174400	-213000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.128380671D+04	3.775179430D+02	-5.992550410D-01	2.181894272D-02	-2.425918417D-05					
1.451245206D-08	-3.596233380D-12		-2.841042565D+04	2.934561769D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.293188730D+05	-4.483030570D+03	1.242199567D+01	-7.463139640D-04	1.332996131D-07					
-1.282710550D-11	5.137997900D-16		-8.518232680D+02	-5.068065510D+01					

CP Gurvich,1991 pt1 p231 pt2 p219.

2 tpis91 C	1.00P	1.00	0.00	0.00	0.00	0.00	0.00	42.9844610	520161.805
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.523940110D+04	7.758828140D+02	-1.453947907D+00	1.397713706D-02	-1.624489706D-05					
9.514083880D-09	-2.210281109D-12		5.792634670D+04	3.311647920D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.449937150D+06	1.688345926D+04	-1.595692200D+01	1.136028761D-02	-2.846541330D-06					
3.379364040D-10	-1.554457397D-14		-4.554517740D+04	1.451324059D+02					

CS Hf:Prinslow,1991. Gurvich,1991 pt1 p206 pt2 p198.

2 g11/01 C	1.00S	1.00	0.00	0.00	0.00	0.00	0.00	44.0757000	278550.078
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.924844120D+04	8.166968100D+02	-1.542998408D+00	1.380324735D-02	-1.574407905D-05					
9.169714930D-09	-2.169700595D-12		2.865182876D+04	3.308541327D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.719574760D+05	2.339201284D+03	1.709390402D+00	1.577178949D-03	-4.146335910D-07					
4.504757080D-11	-5.945457730D-16		1.681020727D+04	1.874048220D+01					

CS2 Gurvich,1991 pt1 p209 pt2 p199.

2 g 6/95 C	1.00S	2.00	0.00	0.00	0.00	0.00	0.00	76.1407000	116700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.613560482D+04	-4.649481470D+02	6.297938790D+00	1.888896706D-03	3.031927747D-07					
-1.737645373D-09	7.793989390D-13		1.477761119D+04	-9.303382130D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.390419724D+06	3.354975500D+03	3.019247723D+00	2.876437543D-03	-9.076812720D-07					
1.374091042D-10	-6.999575570D-15		-1.013898046D+04	1.565113703D+01					

C2 Gurvich,1991 pt1 p9 pt2 p8.

3 tpis91 C	2.00	0.00	0.00	0.00	0.00	0.00	0.00	24.0214000	830457.322
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.559634510D+05	-9.980126440D+03	6.681620370D+01	-1.743432724D-01	2.448523051D-04					
-1.703467580D-07	4.684527730D-11		1.445869634D+05	-3.448229700D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.689267930D+05	3.561092990D+03	-5.064138930D-01	2.945154879D-03	-7.139441190D-07					
8.670657250D-11	-4.076906810D-15		7.681796830D+04	3.339985240D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.315145920D+06	1.365420661D+04	-3.996903670D+00	1.937561376D-03	-1.584446580D-07					
5.520861660D-12	-7.253735340D-17		9.387024990D+03	6.614329920D+01					

C2+ Gurvich,1991 pt1 p14 pt2 p10.

3 tpis91 C	2.00E	-1.00	0.00	0.00	0.00	0.00	0.00	24.0208514	2004775.532
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.913423840D+04	1.347170609D+03	-3.476753160D+00	1.676429424D-02	-1.865908025D-05					
1.091134647D-08	-2.434913818D-12		2.335454800D+05	4.406644620D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.836292810D+06	-6.242062450D+03	2.779245639D+00	6.065865860D-03	-2.452799858D-06					
3.882942500D-10	-2.190639912D-14		2.857447553D+05	7.297383490D-01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.992689800D+07	-2.017309121D+04	6.342227540D+00	6.369922600D-04	-1.036760828D-07					
4.943272920D-12	-7.988804260D-17		4.120857610D+05	-2.112967169D+01					

## Appendix D (continued)

C2- Gurvich,1991 pt1 p15 pt2 p12.

2 tpis91 C	2.00E	1.00	0.00	0.00	0.00	0.00	0.00	24.0219486	480766.904
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.181928660D+05	1.438189710D+03	-3.196131350D+00	1.465548163D-02	-1.545537278D-05					
9.061235610D-09	2.135962274D-12				4.965317790D+04	4.225608880D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.478136250D+06	-1.154145714D+04	1.310143499D+01	-1.862700578D-03	4.006931250D-08					
3.710213600D-11	3.337266870D-15				1.325356168D+05	-6.975964400D+01			

C2CL Gurvich,1991 pt1 p112 pt2 p85.

2 tpis91 C	2.00CL	1.00	0.00	0.00	0.00	0.00	0.00	59.4744000	534083.071
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.725889410D+04	-8.980223610D+02	9.016877150D+00	-6.333782830D-03	1.087060050D-05					
-8.089068920D-09	2.248275223D-12				6.702215700D+04	-2.354893403D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.137368408D+05	-1.630519518D+03	8.623490250D+00	-4.253517860D-04	9.040018640D-08					
-1.007541495D-11	4.570764750D-16				7.171093280D+04	-2.413014598D+01			

C2CL2 Hf:Manion,2002. Gurvich,1991 pt1 p114 pt2 p86.

2 g 5/02 C	2.00CL	2.00	0.00	0.00	0.00	0.00	0.00	94.9268000	226600.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.871169080D+04	-9.336870730D+02	1.119377861D+01	-3.746288200D-03	6.770472560D-06					
-4.910388350D-09	1.299068749D-12	0.000000000D+00	2.948153198D+04	-3.310724640D+01					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.961978472D+05	-2.044286552D+03	1.187529315D+01	-5.115011450D-04	1.072661556D-07					
-1.183411171D-11	5.326498340D-16	0.000000000D+00	3.636799690D+04	-4.000823970D+01					

C2CL3 Gurvich,1991 pt1 p114 pt2 p87.

2 tpis91 C	2.00CL	3.00	0.00	0.00	0.00	0.00	0.00	130.3804000	190271.592
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.675016040D+04	-8.851019640D+02	9.032270550D+00	1.242122796D-02	-1.554614347D-05					
9.513887120D-09	-2.341473263D-12				2.495863399D+04	-1.779070154D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.204028219D+05	-1.072926248D+03	1.378367377D+01	-3.093322915D-04	6.777528950D-08					
-7.727301820D-12	3.566690220D-16				2.431020015D+04	-4.342161815D+01			

C2CL4 Hf: Manion,2002. Gurvich,1991 pt1 p115 pt2 p88.

2 g 5/02 C	2.00CL	4.00	0.00	0.00	0.00	0.00	0.00	165.8322000	-24200.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.746258300D+04	-8.481775630D+02	1.009156110D+01	1.845463613D-02	-2.390899444D-05					
1.514828257D-08	-3.841119320D-12	0.000000000D+00	-1.598288471D+03	-2.368080605D+01					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.001315659D+05	-1.132407598D+03	1.683072470D+01	-3.288792490D-04	7.220907030D-08					
-8.245332690D-12	3.810112780D-16	0.000000000D+00	-2.292799594D+03	-5.980161160D+01					

C2CL6 Hf:Manion,2002. Gurvich,1991 pt1 p117 pt2 p90.

2 g 5/02 C	2.00CL	6.00	0.00	0.00	0.00	0.00	0.00	236.7376000	-148200.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.593451813D+05	-2.606697136D+03	2.028011847D+01	1.769364822D-02	-3.133105185D-05					
2.389395238D-08	-6.893038300D-12	0.000000000D+00	-9.038007640D+03	-7.953073760D+01					
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.577386320D+05	-4.976491240D+02	2.237041989D+01	-1.477759098D-04	3.257546580D-08					
-3.727099210D-12	1.723801704D-16	0.000000000D+00	-2.335223305D+04	-8.381732120D+01					

C2F Gurvich,1991 pt1 p81 pt2 p59.

2 tpis91 C	2.00F	1.00	0.00	0.00	0.00	0.00	0.00	43.0198032	353847.482
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.249797213D+04	-3.483876750D+02	5.755084350D+00	8.528685380D-04	2.353546435D-06					
-2.804737097D-09	9.083575640D-13				4.281525310D+04	-6.437200960D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.898776676D+05	-2.016644658D+03	8.875045710D+00	-5.166841130D-04	1.092094306D-07					
-1.212216787D-11	5.482287680D-16				5.241287920D+04	-2.773089580D+01			

C2FCL Gurvich,1991 pt1 p141 pt2 p113.

2 tpis91 C	2.00F	1.00CL	1.00	0.00	0.00	0.00	0.00	78.4728032	33766.399
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.697675344D+04	-7.414403180D+02	9.629604300D+00	-3.865544930D-04	3.003347997D-06					
-2.710191661D-09	7.737586890D-13				5.500620390D+03	-2.515774889D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.471454890D+05	-2.348461100D+03	1.206875617D+01	-5.804698230D-04	1.212734340D-07					
-1.334214186D-11	5.992556610D-16				1.502061224D+04	-4.252445687D+01			

## Appendix D (continued)

C2FCL3                      Gurvich,1991 pt1 p145 pt2 p119.

2 tpis91 C	2.00F	1.00CL	3.00	0.00	0.00	0	149.3788032	-166000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.237282217D+04	-4.703961840D+02	7.581621790D+00	2.305727066D-02	-2.792144322D-05				
1.679699826D-08	-4.077572440D-12		-2.031333976D+04	-9.274637513D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								18731.914
-2.829505545D+05	-1.473853145D+03	1.707879074D+01	-4.265213390D-04	9.357199850D-08				
-1.067932796D-11	4.933261610D-16		-1.738433314D+04	-6.197054796D+01				

C2F2                      Gurvich,1991 pt1 p82 pt2 p60.

2 tpis91 C	2.00F	2.00	0.00	0.00	0.00	0	62.0182064	-144665.688
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.776313572D+04	-6.113280940D+02	8.663606800D+00	9.156381210D-04	2.363808425D-06				
-2.753750054D-09	8.713935970D-13		-1.649611017D+04	-2.165150307D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								13266.419
4.193890940D+05	-2.715359989D+03	1.230403413D+01	-6.649305540D-04	1.385254301D-07				
-1.520813764D-11	6.819821030D-16		-4.179221940D+03	-4.670386230D+01				

C2F2CL2                      Gurvich,1991 pt1 p143 pt2 p115. Eql mixture of isomers.

2 tpis91 C	2.00F	2.00CL	2.00	0.00	0.00	0	132.9242064	-337837.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.150433214D+05	-2.032113595D+03	-1.119750271D+01	8.342451400D-02	-1.163698616D-04				
7.833092890D-08	-2.070004069D-11		-5.208256810D+04	8.888322147D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								17936.029
-8.702565660D+05	7.264724480D+02	1.530689121D+01	3.045597224D-04	-7.045468040D-08				
8.285924340D-12	-3.898581070D-16		-5.208888710D+04	-4.998300753D+01				

C2F3                      Gurvich,1991 pt1 p83 pt2 p61.

2 tpis91 C	2.00F	3.00	0.00	0.00	0.00	0	81.0166096	-228181.093
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.614775016D+04	2.101767714D+02	2.328625080D+00	2.368943293D-02	-2.416431591D-05				
1.224916093D-08	-2.488670434D-12		-3.028566585D+04	1.699608790D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								14163.567
-1.242603837D+05	-2.137292446D+03	1.455051371D+01	-6.093891980D-04	1.331427672D-07				
-1.515124358D-11	6.984112060D-16		-1.977146179D+04	-5.421039870D+01				

C2F3CL                      Gurvich,1991 pt1 p142 pt2 p114.

2 tpis91 C	2.00F	3.00CL	1.00	0.00	0.00	0	116.4696096	-515200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.122270310D+03	-1.574007092D+02	5.041810290D+00	2.621692321D-02	-2.843001445D-05				
1.537643979D-08	-3.360730670D-12		-6.354049950D+04	2.792301872D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								17128.149
-2.162724659D+05	-2.195103372D+03	1.759605428D+01	-6.282617290D-04	1.374166610D-07				
-1.565004037D-11	7.218309900D-16		-5.515109500D+04	-6.921931824D+01				

C2F4                      Gurvich,1991 pt1 p84 pt2 p62.

2 tpis91 C	2.00F	4.00	0.00	0.00	0.00	0	100.0150128	-659500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.991530070D+04	-1.291088427D+02	4.504229050D+00	2.592029640D-02	-2.630308720D-05				
1.316489777D-08	-2.625017169D-12		-8.090447080D+04	3.274241470D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								16330.554
-1.629915758D+05	-2.603903955D+03	1.788488423D+01	-7.397038010D-04	1.614460340D-07				
-1.835820392D-11	8.457641070D-16		-7.006371660D+04	-7.454165860D+01				

C2F6                      Gurvich,1991 pt1 p86 pt2 p64.

2 g12/99 C	2.00F	6.00	0.00	0.00	0.00	0	138.0118192	-1344000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.795371700D+04	7.998276400D+02	-4.671561810D+00	7.501450990D-02	-9.812116100D-05				
6.319807590D-08	-1.622597311D-11		-1.675211878D+05	5.053759200D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								20272.040
-1.011551484D+06	-9.422140710D+02	2.202553906D+01	-1.314518750D-04	1.866045300D-08				
-3.467118610D-12	2.488311205D-16		-1.657434402D+05	-9.302161150D+01				

C2H                      Ervin, 1990. Jacox,1998. Peric,1990. Kanamori,1988.

2 g 6/01 C	2.00H	1.00	0.00	0.00	0.00	0	25.0293400	566200.482
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.343669487D+04	-5.067970720D+02	7.772107410D+00	-6.512339820D-03	1.030117855D-05				
-5.880147670D-09	1.226901861D-12		6.892269990D+04	-1.871881626D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								10448.682
3.922334570D+06	-1.204751703D+04	1.756172920D+01	-3.655442940D-03	6.987685430D-07				
-6.825162010D-11	2.719262793D-15		1.433266627D+05	-9.561634380D+01				



## Appendix D (continued)

C2HCL Hf:Manion,2002. Gurvich,1991 pt1 p129 pt2 p99.  
 2 g 5/02 C 2.00H 1.00CL 1.00 0.00 0.00 0 60.4820400 226400.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11787.625  
 1.329785007D+05-2.174542126D+03 1.497980854D+01-1.290343389D-02 1.602596678D-05  
 -9.152049510D-09 2.021223607D-12 0.000000000D+00 3.604801320D+04-5.958237870D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11787.625  
 1.152145326D+06-4.461193000D+03 1.281366744D+01-6.797346760D-04 1.151382756D-07  
 -1.046641954D-11 3.949860520D-16 0.000000000D+00 5.233947560D+04-5.320654570D+01

C2HCL3 Hf:Manion,2002. Gurvich,1991 pt1 p134 pt2 p105.  
 2 g 5/02 C 2.00H 1.00CL 3.00 0.00 0.00 0 131.3874400 -17500.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16604.624  
 3.959231250D+04-5.178753580D+02 5.155028770D+00 2.816922486D-02-3.624741720D-05  
 2.392074270D-08-6.362401960D-12 0.000000000D+00-1.534346259D+03 1.209374516D+00  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16604.624  
 6.049254660D+05-4.236992320D+03 1.846273557D+01-8.137195060D-04 1.551211545D-07  
 -1.184559365D-11 6.700932490D-16 0.000000000D+00 1.848285551D+04-7.698368760D+01

C2HF Gurvich,1991 pt1 p99 pt2 p73.  
 2 tps91 C 2.00H 1.00F 1.00 0.00 0.00 0 44.0277432 41692.304  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11445.908  
 9.161169110D+04-1.537245636D+03 1.133665074D+01-4.624729310D-03 5.877985460D-06  
 -2.690992345D-09 3.524719530D-13 1.085902820D+04-4.023994380D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11445.908  
 1.234347179D+06-4.819581960D+03 1.302337752D+01-7.495435820D-04 1.285452942D-07  
 -1.184559365D-11 4.536784760D-16 3.236811710D+04-5.640793820D+01

C2HFCL2 Gurvich,1991 pt1 p155 pt2 p133. Eql mixture of isomers.  
 2 tps91 C 2.00H 1.00F 1.00CL 2.00 0.00 0 114.9337432 -168648.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16259.290  
 3.117399823D+04-1.369505457D+02 1.176399869D+00 4.080776600D-02-5.418137800D-05  
 3.613600660D-08-9.625862350D-12 -2.115142871D+04 2.146433160D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16259.290  
 4.071243520D+05-3.808204520D+03 1.821144050D+01-7.278966060D-04 1.381532849D-07  
 -1.405342513D-11 5.920009720D-16 -2.676849943D+03-7.567353567D+01

C2HF2CL Gurvich,1991 pt1 p153 pt2 p129. 1,1 cis & trans in equil.  
 2 tps91 C 2.00H 1.00F 2.00CL 1.00 0.00 0 98.4791464 -333654.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15262.754  
 1.704437675D+05-1.667236861D+03 4.788788500D+00 4.444830010D-02-7.322197700D-05  
 5.629347550D-08-1.654638029D-11 -3.291809760D+04-5.788593640D+00  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15262.754  
 5.830374700D+05-3.810317410D+03 1.799003171D+01-5.888210860D-04 1.002861284D-07  
 -9.149788100D-12 3.459985160D-16 -2.205875409D+04-7.590948533D+01

C2HF3 Gurvich,1991 pt1 p105 pt2 p79.  
 2 tps91 C 2.00H 1.00F 3.00 0.00 0.00 0 82.0245496 -491000.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14327.512  
 -1.410969036D+04 3.687624920D+02-1.144797568D+00 3.956306020D-02-4.602001360D-05  
 2.785149385D-08-6.903760080D-12 -6.226410330D+04 3.289661690D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14327.512  
 6.917413780D+05-5.260301640D+03 1.915276614D+01-1.072493938D-03 2.099276744D-07  
 -2.195126633D-11 9.472702400D-16 -3.247640210D+04-8.750456950D+01

C2H2,acetylene Hf:TRC(10/93) w-3040. Gurvich,1991 pt1 p47 pt2 p39.  
 2 g 1/91 C 2.00H 2.00 0.00 0.00 0.00 0 26.0372800 228200.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10005.839  
 1.598112089D+05-2.216644118D+03 1.265707813D+01-7.979651080D-03 8.054992750D-06  
 -2.433307673D-09-7.529233180D-14 3.712619060D+04-5.244338900D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10005.839  
 1.713847410D+06-5.929106660D+03 1.236127943D+01 1.314186993D-04-1.362764431D-07  
 2.712655786D-11-1.302066204D-15 6.266578970D+04-5.818960590D+01

C2H2,vinylidene Chen,1989. Osamura,1981.  
 2 g 5/01 C 2.00H 2.00 0.00 0.00 0.00 0 26.0372800 414788.368  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10874.168  
 -1.466042239D+04 2.789475593D+02 1.276229776D+00 1.395015463D-02-1.475702649D-05  
 9.476298110D-09-2.567602217D-12 4.736110180D+04 1.658225704D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10874.168  
 1.940838725D+06-6.892718150D+03 1.339582494D+01-9.368968670D-04 1.470804368D-07  
 -1.220040365D-11 4.122391660D-16 9.107112930D+04-6.337502930D+01

## Appendix D (continued)

C2H2CL2                      Gurvich,1991 pt1 p130 pt2 p101. 1,1 cis & trans in equil.  
 2 tpis91 C    2.00H    2.00CL    2.00    0.00    0.00 0    96.9432800    3410.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14882.477  
 -1.203724514D+04 4.629031190D+02-1.318184584D+00 3.930449600D-02-4.851529020D-05  
 3.178411460D-08-8.476938410D-12                      -3.251806860D+03 3.489218118D+01  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14882.477  
 1.561121185D+06-7.358096350D+03 2.011869185D+01-1.310978834D-03 2.411885716D-07  
 -2.384166740D-11 9.785415750D-16                      4.122200900D+04-9.550252712D+01

C2H2FCL                      Gurvich,1991 pt1 p150 pt2 p125. 1,1 cis & trans in equil.  
 2 tpis91 C    2.00H    2.00F    1.00CL    1.00    0.00 0    80.4886832    -165082.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13469.313  
 2.260154427D+05-2.557428772D+03 9.236241200D+00 2.879408894D-02-5.163975470D-05  
 4.252191030D-08-1.311612713D-11                      -8.180627840D+03-3.234787581D+01  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13469.313  
 1.527690968D+06-6.689712230D+03 1.950553830D+01-1.040920895D-03 1.780587502D-07  
 -1.633098515D-11 6.213465560D-16                      1.705266451D+04-9.194078301D+01

C2H2F2                      Gurvich,1991 pt1 p101 pt2 p75. 1,1 cis & trans in equil.  
 2 tpis91 C    2.00H    2.00F    2.00    0.00    0.00 0    64.0340864    -336400.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12479.683  
 5.702935810D+04-6.762860400D+02 4.117411710D+00 1.822618762D-02-6.861331540D-06  
 -3.295756740D-09 2.180965597D-12                      -3.838650780D+04 1.487528685D+00  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12479.683  
 -8.227192750D+05-2.915718833D+03 1.830163995D+01-1.039630129D-03 2.546725128D-07  
 -3.157578705D-11 1.551540960D-15                      -3.110028589D+04-8.400834700D+01

CH2CO, ketene                      Wagman,1982. Moore,1963.  
 2 g 7/00 C    2.00H    2.00O    1.00    0.00    0.00 0    42.0366800    -47700.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    11797.746  
 3.503274040D+04-4.001693250D+02 3.691806430D+00 1.589408702D-02-1.733190594D-05  
 1.161219965D-08-3.313412960D-12                      -5.014866400D+03 2.848266196D+00  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    11797.746  
 2.015132200D+06-8.200240060D+03 1.759005013D+01-1.460345107D-03 2.684671350D-07  
 -2.651382523D-11 1.087131348D-15                      4.200517260D+04-8.836222940D+01

O(CH)2O                      Glyoxal. Dorofeeva,2001. Hubner,1997. Zeleznik,2002.  
 2 g 3/02 C    2.00H    2.00O    2.00    0.00    0.00 0    58.0360800    -212000.000  
 200.000    1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13682.443  
 -2.292459698D+05 3.724098050D+03-1.893769993D+01 7.511744140D-02-8.083855420D-05  
 4.358233190D-08-9.364539330D-12 0.000000000D+00-4.454486010D+04 1.327028760D+02  
 1000.000    6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13682.443  
 2.678063593D+05-4.436617480D+03 1.781696797D+01-7.097173780D-04 1.272621878D-07  
 -1.237226678D-11 5.025057520D-16 0.000000000D+00-4.479608280D+03-8.156700640D+01

HO(CO)2OH                      Oxalic Acid, HO-CO-CO-OH. Dorofeeva,2001.  
 2 srd 01 C    2.00H    2.00O    4.00    0.00    0.00 0    90.0348800    -731800.000  
 200.000    1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17321.662  
 3.072513274D+04 3.916174690D+02 3.178388640D+00 3.741289750D-02-4.009753960D-05  
 2.288662646D-08-5.386771550D-12 0.000000000D+00-8.797942550D+04 9.751091370D+00  
 1000.000    6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17321.662  
 1.805560696D+06-9.240333150D+03 2.625742604D+01-1.418458557D-03 2.526840574D-07  
 -2.521005198D-11 1.040036111D-15 0.000000000D+00-3.754286460D+04-1.326879788D+02

C2H3, vinyl                      Radical. Ervin,1990.  
 2 g 7/01 C    2.00H    3.00    0.00    0.00    0.00 0    27.0452200    299686.817  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    10521.791  
 -3.347896870D+04 1.064104103D+03-6.403857060D+00 3.934515480D-02-4.760046090D-05  
 3.170071350D-08-8.633406430D-12                      3.039122649D+04 5.809226180D+01  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    10521.791  
 2.718080093D+06-1.030956829D+04 1.836579807D+01-1.580131153D-03 2.680594939D-07  
 -2.439003999D-11 9.209096390D-16                      9.765055590D+04-9.760086860D+01

CH2Br-COOH                      Bromoacetic Acid. Dorofeeva,2001.  
 2 srd 01 C    2.00H    3.00BR    1.00O    2.00    0.00 0    138.9480200    -383500.000  
 200.000    1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    16862.437  
 -7.832484790D+04 1.648865353D+03-9.349533630D+00 6.879635440D-02-8.374880770D-05  
 5.406038420D-08-1.423159923D-11 0.000000000D+00-5.541187620D+04 8.165423200D+01  
 1000.000    6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    16862.437  
 2.486349850D+06-1.140256346D+04 2.756020307D+01-1.843187010D-03 3.265392740D-07  
 -3.122663159D-11 1.223452495D-15 0.000000000D+00 1.837013127D+04-1.420040888D+02

## Appendix D (continued)

C2H3CL Hf:Manion,2002. Gurvich,1991 pt1 p129 pt2 p100.  
 2 g 5/02 C 2.00H 3.00CL 1.00 0.00 0.00 0 62.4979200 22000.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11819.647  
 -1.688895457D+04 8.545104550D+02-6.514967550D+00 4.944681930D-02-6.117756670D-05  
 4.067293850D-08-1.101392611D-11 0.000000000D+00-2.069321321D+03 5.928434500D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11819.647  
 2.456176938D+06-1.047452327D+04 2.178736181D+01-1.816891849D-03 3.296369950D-07  
 -3.214395690D-11 1.302254061D-15 0.000000000D+00 6.346228700D+04-1.149890578D+02

CH2CL-COOH Chloroacetic Acid. Dorofeeva,2001.  
 2 srd 01 C 2.00H 3.00CL 1.000 2.00 0.00 0 94.4967200 -427600.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16513.941  
 -1.122506518D+05 2.168288658D+03-1.227791286D+01 7.514388250D-02-9.083158770D-05  
 5.812364190D-08-1.518247503D-11 0.000000000D+00-6.314314550D+04 9.694389590D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16513.941  
 2.472883176D+06-1.152275963D+04 2.766275606D+01-1.886430963D-03 3.361776050D-07  
 -3.213272250D-11 1.273275883D-15 0.000000000D+00 1.370387108D+04-1.443191401D+02

C2H3F Gurvich,1991 pt1 p100 pt2 p74.  
 2 tpis91 C 2.00H 3.00F 1.00 0.00 0.00 0 46.0436232 -140100.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11335.928  
 -4.579134960D+04 1.411541724D+03-1.021500877D+01 5.775816570D-02-7.080677490D-05  
 4.640850760D-08-1.240455865D-11 -2.402788827D+04 7.860828390D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11335.928  
 2.478832340D+06-1.075932307D+04 2.194796688D+01-1.869114110D-03 3.395280670D-07  
 -3.315382930D-11 1.345081799D-15 4.563455550D+04-1.180410277D+02

CH3CN Acetonitrile. TRC(6/93) w9270. Koga,1984. Pavone,1990.  
 2 g 9/00 C 2.00H 3.00N 1.00 0.00 0.00 0 41.0519200 66430.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12093.688  
 -9.965988380D+04 1.739278534D+03-7.898420820D+00 4.294894320D-02-4.499973880D-05  
 2.717105086D-08-7.026117590D-12 -1.461161333D+03 6.852508274D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12093.688  
 2.923231393D+06-1.233792258D+04 2.324477222D+01-2.411565845D-03 4.622157170D-07  
 -4.740601240D-11 2.010639467D-15 8.058565550D+04-1.292249102D+02

CH3CO,acetyl Radical. Hf:Niiranen,1992. Nimlos,1989.  
 2 g 6/96 C 2.00H 3.00O 1.00 0.00 0.00 0 43.0446200 -10000.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13036.467  
 -7.193894130D+04 1.464465167D+03-6.632276130D+00 4.108468380D-02-4.226256640D-05  
 2.485766819D-08-6.292558480D-12 -9.309370810D+03 6.422897620D+01  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13036.467  
 2.485388150D+06-1.120714204D+04 2.277525438D+01-2.314260550D-03 4.536189170D-07  
 -4.742635550D-11 2.044663903D-15 6.380088410D+04-1.215350925D+02

C2H4 TRC(4/88) w2600. Chao,1975. Knippers,1985.  
 2 g 1/00 C 2.00H 4.00 0.00 0.00 0 28.0531600 52500.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10518.689  
 -1.163605836D+05 2.554851510D+03-1.609746428D+01 6.625779320D-02-7.885081860D-05  
 5.125224820D-08-1.370340031D-11 -6.176191070D+03 1.093338343D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10518.689  
 3.408763670D+06-1.374847903D+04 2.365898074D+01-2.423804419D-03 4.431395660D-07  
 -4.352683390D-11 1.775410633D-15 8.820429380D+04-1.371278108D+02

C2H4O,ethylen-o Ethylene Oxide. Shimanouchi,1972. Chase,1998 9/65.  
 2 g 8/88 C 2.00H 4.00O 1.00 0.00 0.00 0 44.0525600 -52634.720  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10830.615  
 -1.728233345D+05 3.816678800D+03-2.629851977D+01 1.014103162D-01-1.240578373D-04  
 8.034040350D-08-2.120942544D-11 -2.437519333D+04 1.654885056D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10830.615  
 3.151809957D+06-1.423646316D+04 2.708080476D+01-2.606238456D-03 4.853891930D-07  
 -4.852144760D-11 2.011778721D-15 7.662561440D+04-1.563952401D+02

CH3CHO,ethanal Hf:TRC (6/78) w5300. Chao,1986.  
 2 g 8/88 C 2.00H 4.00O 1.00 0.00 0.00 0 44.0525600 -166190.000  
 200.000 1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12896.716  
 -1.373904369D+05 2.559937679D+03-1.340470172D+01 5.922128620D-02-6.240006050D-05  
 3.703324410D-08-9.342697410D-12 -3.318731310D+04 1.007417652D+02  
 1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12896.716  
 3.321176590D+06-1.449719957D+04 2.708421279D+01-2.879320054D-03 5.556309920D-07  
 -5.732674880D-11 2.443965239D-15 6.507755640D+04-1.536236027D+02

## Appendix D (continued)

CH<sub>3</sub>COOH                      Acetic Acid. Chao,1978.  
 2 g 6/00 C    2.00H    4.000    2.00    0.00    0.00 0    60.0519600    -432249.040  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13597.391  
 -3.219191980D+04 1.196329795D+03-8.705824020D+00 5.696257590D-02-5.757887160D-05  
               3.352115220D-08-8.614438230D-12                      -5.840112870D+04 7.282413920D+01  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13597.391  
 2.103514223D+06-1.467822192D+04 3.382802830D+01-5.694858680D-03 1.343221353D-06  
 -1.606041158D-10 7.652794250D-15                      2.924228407D+04-1.935278850D+02

OHCH<sub>2</sub>COOH                      Glycolic Acid. Dorofeeva,2001.  
 2 srd 01 C    2.00H    4.000    3.00    0.00    0.00 0    76.0513600    -583000.000  
               200.000    1000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17007.039  
 -3.138978580D+05 5.693068770D+03-3.685160290D+01 1.563502811D-01-2.039487993D-04  
               1.340232412D-07-3.509130260D-11 0.000000000D+00-9.801640090D+04 2.269492355D+02  
               1000.000    6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17007.039  
 1.946628253D+06-9.804020200D+03 2.844111243D+01-7.876404750D-04 6.416275950D-08  
 1.069321262D-12-3.237178280D-16 0.000000000D+00-1.694650470D+04-1.474109363D+02

C<sub>2</sub>H<sub>5</sub>                              Chen,1990.  
 2 g 7/00 C    2.00H    5.00    0.00    0.00    0.00 0    29.0611000    118658.240  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12185.226  
 -1.411312551D+05 2.714285088D+03-1.534977725D+01 6.451672580D-02-7.259143960D-05  
               4.599116010D-08-1.218367535D-11                      5.981418840D+02 1.090966520D+02  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12185.226  
 4.169220400D+06-1.662982142D+04 2.795442134D+01-3.051715761D-03 5.685160040D-07  
 -5.682863600D-11 2.355648561D-15                      1.137010087D+05-1.639357995D+02

C<sub>2</sub>H<sub>5</sub>Br                              Bromoethane. TRC(6/79) tuvuw7650.  
 2 n 6/79 C    2.00H    5.00BR    1.00    0.00    0.00 0    108.9651000    -63600.000  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13569.000  
 -1.374172662D+05 2.861429418D+03-1.824108956D+01 8.566230600D-02-1.047174473D-04  
               6.906074570D-08-1.862276022D-11                      -2.198480205D+04 1.258435579D+02  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13569.000  
 2.378649403D+06-1.267033647D+04 2.777558646D+01-2.010898783D-03 4.436083410D-07  
 -5.348198090D-11 2.639835850D-15                      6.414062050D+04-1.528277085D+02

C<sub>2</sub>H<sub>6</sub>                              Ethane. Pamidimukkala,1982.  
 2 g 7/00 C    2.00H    6.00    0.00    0.00    0.00 0    30.0690400    -83851.544  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    11891.594  
 -1.862044161D+05 3.406191860D+03-1.951705092D+01 7.565835590D-02-8.204173220D-05  
               5.061135800D-08-1.319281992D-11                      -2.702932890D+04 1.298140496D+02  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    11891.594  
 5.025782130D+06-2.033022397D+04 3.322552930D+01-3.836703410D-03 7.238405860D-07  
 -7.319182500D-11 3.065468699D-15                      1.115963950D+05-2.039410584D+02

CH<sub>3</sub>N<sub>2</sub>CH<sub>3</sub>                              Azomethane. Pamidumukkala,1982.  
 2 g 8/88 C    2.00H    6.00N    2.00    0.00    0.00 0    58.0824400    148699.360  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    16524.999  
 -3.738492320D+05 5.880453130D+03-2.986398524D+01 1.087380861D-01-1.167950177D-04  
               6.916894890D-08-1.719950055D-11                      -1.189984084D+04 1.948246321D+02  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    16524.999  
 4.993357090D+06-2.160996161D+04 3.964449920D+01-4.196450110D-03 8.023361980D-07  
 -8.212260020D-11 3.477237440D-15                      1.449962610D+05-2.372109745D+02

C<sub>2</sub>H<sub>5</sub>OH                              Hf:TRC(6/87) w5030. Chao,1986.  
 2 g 8/88 C    2.00H    6.000    1.00    0.00    0.00 0    46.0684400    -234950.000  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14541.926  
 -2.342791392D+05 4.479180550D+03-2.744817302D+01 1.088679162D-01-1.305309334D-04  
               8.437346400D-08-2.234559017D-11                      -5.022229000D+04 1.764829211D+02  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14541.926  
 4.694817650D+06-1.929798213D+04 3.447584040D+01-3.236165980D-03 5.784947720D-07  
 -5.564600270D-11 2.226226400D-15                      8.601622710D+04-2.034801732D+02

CH<sub>3</sub>OCH<sub>3</sub>                              Dimethyl ether. Hf:TRC(6/91) w6040. Chao,1986.  
 2 g 7/00 C    2.00H    6.000    1.00    0.00    0.00 0    46.0684400    -184110.000  
               200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14354.379  
 -2.693103242D+05 4.300709710D+03-2.152788028D+01 8.131833390D-02-8.295671320D-05  
               4.801911510D-08-1.188699808D-11                      -4.410237090D+04 1.467666934D+02  
               1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14354.379  
 4.933577190D+06-2.083094065D+04 3.629050610D+01-4.108351640D-03 7.903220310D-07  
 -8.131435630D-11 3.458166110D-15                      1.013301012D+05-2.185447466D+02

## Appendix D (continued)

CH3O2CH3      Dimethyl peroxide, CH3-O-O-CH3. Dorofeeva,2001.

2	srd	01	C	2.00H	6.000	2.00	0.00	0.00	0.00	0	62.0678400	-125500.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		17153.436
-2.285784757D+05	3.820142570D+03	-1.976647823D+01	8.840743860D-02	-9.641284560D-05								
5.907200830D-08	-1.526491225D-11	0.000000000D+00	-3.492016960D+04	1.386769151D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		17153.436
5.316368470D+06	-2.221267874D+04	4.034335090D+01	-4.612748090D-03	8.792987200D-07								
-9.0682221190D-11	3.865664890D-15	0.000000000D+00	1.161596028D+05	-2.395296055D+02								

CNC      Hf:Gurvich,1991 pt1 p222. Jacox,1998 p173.

2	g	7/00	C	2.00N	1.00	0.00	0.00	0.00	0	38.0281000	804596.472	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		11038.524	
-1.696281385D+04	9.837891630D+01	3.812662940D+00	5.346894230D-03	-2.473598508D-06								
-3.730564220D-10	4.481756860D-13		9.480072570D+04	5.553165572D+00								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		11038.524	
7.948674890D+04	-1.344786906D+03	8.309986460D+00	-2.220105361D-04	1.753683113D-08								
2.545998719D-12	-2.645649117D-16		1.023187495D+05	-2.259793940D+01								

CNC      CNC radical. Gurvich,1991 pt1 p221 pt2 p209.

2	tpis	91	C	2.00N	1.00	0.00	0.00	0.00	0	38.0281000	684914.559	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		11356.611	
-7.075192710D+04	1.007523898D+03	-1.576789967D+00	2.052532634D-02	-2.278935009D-05								
1.283362343D-08	-2.933174091D-12		7.613324850D+04	3.487094132D+01								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		11356.611	
-9.031313560D+04	-8.313236500D+02	8.114735950D+00	-2.447691991D-04	5.397508770D-08								
-6.183984860D-12	2.865172411D-16		8.451833600D+04	-2.102937255D+01								

OCCN      Cyanooxomethyl radical. Dorofeeva,2001.

2	srd	01	C	2.00N	1.000	1.00	0.00	0.00	0	54.0275400	210000.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13594.351
2.428801276D+04	-5.525864620D+02	8.587838170D+00	-3.379387770D-03	1.119841826D-05								
-1.008408077D-08	3.086448824D-12	0.000000000D+00	2.599620072D+04	-1.659592359D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13594.351
9.359131680D+05	-4.441082290D+03	1.368959297D+01	-1.647530917D-03	3.819873440D-07								
-3.945161000D-11	1.509598839D-15	0.000000000D+00	4.951222780D+04	-5.417089680D+01								

C2N2      Gurvich,1979 pt1 p195 pt2 p220.

2	tpis	79	C	2.00N	2.00	0.00	0.00	0.00	0	52.0348000	309100.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12715.153	
1.082404484D+05	-1.928137871D+03	1.553891898D+01	-1.821159329D-02	2.778840840D-05								
-1.899434373D-08	4.949677720D-12		4.449097590D+04	-6.090964741D+01								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12715.153	
7.934423720D+05	-3.997376270D+03	1.314497430D+01	-8.747782000D-04	2.059156733D-07								
-2.200469389D-11	9.974485770D-16		5.863632300D+04	-5.473201251D+01								

C2O      Hf:Gurvich,1991 pt1 p31. Jacox,1998.

2	g	8/00	C	2.000	1.00	0.00	0.00	0.00	0	40.0208000	291038.666	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		10485.718	
-3.959929420D+03	-1.117516348D+02	4.593960060D+00	3.710602020D-03	-7.014760180D-07								
-1.371129839D-09	7.123854000D-13		3.410109740D+04	4.622805600D-01								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		10485.718	
-6.348056590D+05	1.184133091D+03	4.879173340D+00	1.757538773D-03	-3.957552270D-07								
3.989179940D-11	-1.546043135D-15		2.489803938D+04	9.809040590D-01								

C2S2      TRC(6/01) p8150, tuvw-8150.

2	n	6/01	C	2.00S	2.00	0.00	0.00	0.00	0	88.1514000	376660.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13760.000	
4.192544750D+04	-9.776562320D+02	1.085003376D+01	-4.423407890D-03	1.067980519D-05								
-8.781148100D-09	2.538862361D-12		4.789590500D+04	-3.097681854D+01								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13760.000	
8.629908790D+05	-4.325413740D+03	1.460010162D+01	-1.460638433D-03	2.778253364D-07								
-2.755649209D-11	1.105350739D-15		6.839748750D+04	-5.986379853D+01								

C3      Gurvich,1979 pt2 p23.

3	tpis	79	C	3.00	0.00	0.00	0.00	0.00	0	36.0321000	839948.646	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12109.146	
-4.354614480D+04	6.660183220D+02	1.451033157D+00	7.434513120D-03	-3.810152990D-06								
-2.336961396D-11	4.407054530D-13		9.635170200D+04	2.025173297D+01								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12109.146	
4.508098930D+06	-1.461033761D+04	2.281974644D+01	-8.544340610D-03	2.146069341D-06								
-2.103867761D-10	6.351589060D-15		1.911976065D+05	-1.271869723D+02								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12109.146	
1.539589859D+08	-2.089057498D+05	7.681111210D+01	-8.939056190D-03	5.594033240D-07								
-1.743774353D-11	2.181541208D-16		1.650801763D+06	-6.081693320D+02								

## Appendix D (continued)

C3H3,1-propynyl TRC(4/98) tuvw3140.

2 n 4/98 C	3.00H	3.00	0.00	0.00	0.00	0.00	0.00	39.0559200	450000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.505859350D+04	1.350858921D+03	-5.825433930D+00	3.756610480D-02	-3.734903340D-05					
2.117676603D-08	-5.139113250D-12						4.656510530D+04	5.781477550D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.550654870D+06	-1.640574172D+04	2.712605991D+01	-4.474600380D-03	1.037712415D-06					
-1.250211369D-10	6.026582050D-15						1.534087662D+05	-1.565931809D+02	

C3H3,2-propynyl TRC(4/98) tuvw3140.

2 n 4/98 C	3.00H	3.00	0.00	0.00	0.00	0.00	0.00	39.0559200	331800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.188578320D+04	-8.909578670D+02	6.347558820D+00	1.633173115D-02	-1.949975695D-05					
1.417349778D-08	-4.199866320D-12						4.271785830D+04	-1.231400729D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.989723833D+06	-1.118954446D+04	2.222225052D+01	-2.068106902D-03	4.121883640D-07					
-4.438980590D-11	1.970824701D-15						1.061878289D+05	-1.186744583D+02	

C3H4,allene TRC(4/84) w2750. Shimanouchi,1972 p115. Butcher,1973a.

2 g 2/00 C	3.00H	4.00	0.00	0.00	0.00	0.00	0.00	40.0638600	190920.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.645155745D+04	9.629457810D+02	-7.532326680D+00	5.518219110D-02	-6.733585120D-05					
4.532709050D-08	-1.251837614D-11						1.772494269D+04	6.151969760D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.479355100D+06	-1.430412453D+04	2.702534756D+01	-2.557412369D-03	4.706646750D-07					
-4.651688070D-11	1.908219044D-15						1.072312354D+05	-1.548846158D+02	

C3H4,propyne Hf:TRC(10/93) w3040. Trambarulo,1950. Shimanouchi,1972.

2 g 1/00 C	3.00H	4.00	0.00	0.00	0.00	0.00	0.00	40.0638600	184900.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.563884400D+04	8.328139100D+02	-4.073759440D+00	4.113929610D-02	-4.470444950D-05					
2.847458197D-08	-7.695298240D-12						1.710206236D+04	4.516720950D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.710441420D+06	-1.489145507D+04	2.732397127D+01	-2.645264770D-03	4.858300350D-07					
-4.794128480D-11	1.964338121D-15						1.104898462D+05	-1.567992462D+02	

C3H4,cyclo- Dorofeeva,1986.

2 g 5/90 C	3.00H	4.00	0.00	0.00	0.00	0.00	0.00	40.0638600	277100.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.969520627D+04	1.505379338D+03	-1.418206573D+01	7.642632960D-02	-9.765583660D-05					
6.612003820D-08	-1.811251145D-11						2.625631782D+04	9.604631890D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.168399580D+06	-1.371044699D+04	2.664303646D+01	-2.420408050D-03	4.427994130D-07					
-4.351820200D-11	1.775948955D-15						1.133683702D+05	-1.522619086D+02	

C3H5,allyl Radical. Burcat,2001 p58.

2 g 3/01 C	3.00H	5.00	0.00	0.00	0.00	0.00	0.00	41.0718000	163594.400
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.315996140D+04	1.441600907D+03	-1.197014426D+01	7.319796460D-02	-9.066357850D-05					
6.077059450D-08	-1.658826363D-11						1.232157460D+04	8.563173240D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.094570590D+06	-1.676676186D+04	3.123006342D+01	-2.885449982D-03	5.211343540D-07					
-5.058284220D-11	2.039932554D-15						1.185720481D+05	-1.823070197D+02	

C3H6,propylene Hf:TRC(4/88) w2600. Chao,1975.

2 g 2/00 C	3.00H	6.00	0.00	0.00	0.00	0.00	0.00	42.0797400	20000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.912462174D+05	3.542074240D+03	-2.114878626D+01	8.901484790D-02	-1.001429154D-04					
6.267959390D-08	-1.637870781D-11						-1.529961824D+04	1.407641382D+02	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.017620340D+06	-2.086084035D+04	3.644156340D+01	-3.881191170D-03	7.278677190D-07					
-7.321204500D-11	3.052176369D-15						1.261245355D+05	-2.195715757D+02	

C3H6,cyclo- Dorofeeva,1986. Butcher,1973b.

2 g 1/00 C	3.00H	6.00	0.00	0.00	0.00	0.00	0.00	42.0797400	53300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.565787770D+05	4.111129870D+03	-3.233447460D+01	1.306337881D-01	-1.645563833D-04					
1.095708326D-07	-2.956394783D-11						-1.245271686D+04	1.931559109D+02	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.785000670D+06	-2.042118175D+04	3.631495780D+01	-3.561319440D-03	6.476241240D-07					
-6.328430100D-11	2.568705857D-15						1.268274126D+05	-2.223729099D+02	

## Appendix D (continued)

C3H6O, propylox TRC(6/84) w6150. Swalen, 1957. Oetting, 1964. Villarreal, 1975.

2 g 6/01 C	3.00H	6.000	1.00	0.00	0.00	0	58.0791400	-93720.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.292808804D+05	4.495750540D+03	-2.941117945D+01	1.213113827D-01	-1.440060464D-04				
9.202051750D-08	-2.416278343D-11		-3.317697210D+04	1.846878218D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.789729990D+06	-2.106895971D+04	3.954647730D+01	-3.910929980D-03	7.325531510D-07				
-7.357085970D-11	3.060618500D-15		1.120344540D+05	-2.372004192D+02				

C3H6O, acetone Chao, 1986. Chao, 1976.

2 g 6/97 C	3.00H	6.000	1.00	0.00	0.00	0	58.0791400	-217149.600
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.277802525D+05	4.215280010D+03	-2.415785316D+01	9.907483320D-02	-1.084940903D-04				
6.583355960D-08	-1.676046146D-11		-4.726243940D+04	1.607926432D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.001601920D+06	-2.170155542D+04	3.964493990D+01	-4.179945050D-03	7.962429530D-07				
-8.122558050D-11	3.428780960D-15		1.015145028D+05	-2.368533477D+02				

C3H6O, propanal Hf:TRC(6/78) w5300. Chao, 1986. Frankiss, 1974.

2 g 1/02 C	3.00H	6.000	1.00	0.00	0.00	0	58.0791400	-186000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.655781702D+05	4.250640450D+03	-2.109249262D+01	9.194256120D-02	-1.004653044D-04				
6.133314820D-08	-1.576298535D-11	0.000000000D+00	-4.450371050D+04	1.456678605D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.830933490D+06	-2.075451152D+04	3.924855180D+01	-4.095514000D-03	7.881692160D-07				
-8.107684080D-11	3.437105430D-15	0.000000000D+00	9.944937880D+04	-2.316690627D+02				

C3H7, n-propyl Radical. Tsang, 1985.

2 g 7/01 C	3.00H	7.00	0.00	0.00	0.00	0	43.0876800	100500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.895337073D+05	3.949517260D+03	-2.606216089D+01	1.121920441D-01	-1.365292213D-04				
9.023662720D-08	-2.441056990D-11		-7.227877440D+03	1.673705556D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.646512940D+06	-2.291087136D+04	3.987275180D+01	-4.106232870D-03	7.562557770D-07				
-7.478263020D-11	3.068983677D-15		1.483006853D+05	-2.403781190D+02				

C3H7, i-propyl Radical. Tsang, 1985.

2 g 9/85 C	3.00H	7.00	0.00	0.00	0.00	0	43.0876800	93300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.952063445D+05	5.294432300D+03	-3.105287013D+01	1.143871563D-01	-1.291752393D-04				
8.057843760D-08	-2.093908432D-11		-1.476815514D+04	1.988082360D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.807002520D+06	-2.411219997D+04	4.085288400D+01	-4.517851330D-03	8.499427170D-07				
-8.573514340D-11	3.583383960D-15		1.546504050D+05	-2.487098372D+02				

C3H8 Hf:TRC(10/85) w1350. Chao, 1973.

2 g 2/00 C	3.00H	8.00	0.00	0.00	0.00	0	44.0956200	-104680.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.433144337D+05	4.656270810D+03	-2.939466091D+01	1.188952745D-01	-1.376308269D-04				
8.814823910D-08	-2.342987994D-11		-3.540335270D+04	1.841749277D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.420731680D+06	-2.659791134D+04	4.534356840D+01	-5.020663920D-03	9.471216940D-07				
-9.575405230D-11	4.009672880D-15		1.455582459D+05	-2.818374734D+02				

C3H8O, 1propanol Hf:TRC(6/87) w5030. Chao, 1986.

2 g 2/00 C	3.00H	8.000	1.00	0.00	0.00	0	60.0950200	-255200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.616973337D+05	5.192376660D+03	-3.296481160D+01	1.354568128D-01	-1.593156164D-04				
1.019498160D-07	-2.688552974D-11		-5.612854350D+04	2.085024431D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.308672120D+06	-2.642210376D+04	4.715112590D+01	-4.642511930D-03	8.593465360D-07				
-8.682091820D-11	3.642224010D-15		1.255003155D+05	-2.859463804D+02				

C3H8O, 2propanol Hf:TRC(6/87) w5030. Chao, 1986.

2 g 2/00 C	3.00H	8.000	1.00	0.00	0.00	0	60.0950200	-272700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.386510240D+05	6.106048000D+03	-3.791418040D+01	1.530494531D-01	-1.864354461D-04				
1.213257738D-07	-3.220433490D-11		-6.279959350D+04	2.334322610D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.001074750D+06	-2.505876830D+04	4.622096120D+01	-4.272466310D-03	7.693678770D-07				
-7.450584840D-11	2.998959935D-15		1.148518732D+05	-2.796132222D+02				

## Appendix D (continued)

CNCOCN Oxopropanedinitrile, NC-CO-CN. Dorofeeva, 2001.

2	srd	01	C	3.00N	2.000	1.00	0.00	0.00	0.00	0	80.0449800	247500.000
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		17147.758
1.131052075D+05	-1.978834961D+03	1.626886206D+01	-8.330803440D-03	1.884127045D-05								
-1.530681289D-08	4.418125300D-12	0.000000000D+00	3.680261740D+04	-5.963327280D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		17147.758
7.000522440D+05	-5.086002010D+03	1.946753490D+01	-1.302852727D-03	2.753600750D-07								
-3.056290852D-11	1.382140838D-15	0.000000000D+00	5.539338880D+04	-8.627550860D+01								

C3OS TRC(6/01) p8150, tuvw-8150.

2	n	6/01	C	3.00O	1.00S	1.00	0.00	0.00	0	84.0965000	157330.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15720.000
1.173396837D+05	-2.154246274D+03	1.739096818D+01	-1.606951508D-02	2.815913738D-05								
-2.144517776D-08	6.117883960D-12		2.690975728D+04	-6.715503804D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15720.000
4.650964090D+05	-3.653583100D+03	1.589374854D+01	-7.274431680D-04	1.507932631D-07								
-1.250975180D-11	2.879103391D-16		3.664221650D+04	-6.509079314D+01								

C3O2 Hf:Chase, 1998 p690 6/68. Shimanouchi, 1977 p1083.

2	g	7/88	C	3.00O	2.00	0.00	0.00	0.00	0	68.0309000	-93638.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15084.983
1.579873382D+05	-2.529493506D+03	1.801761578D+01	-1.786032042D-02	2.978671986D-05								
-2.182900022D-08	6.013797220D-12		-1.121054014D+03	-7.277721170D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15084.983
6.968699890D+05	-4.624733190D+03	1.663905725D+01	-1.175486554D-03	2.478106444D-07								
-2.745165984D-11	1.239566766D-15		1.252580069D+04	-7.275968780D+01								

C3S2 TRC(6/01) p8150, tuvw-8150.

2	n	6/01	C	3.00S	2.00	0.00	0.00	0.00	0	100.1621000	412500.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15990.000
9.328308590D+04	-1.860679192D+03	1.613667767D+01	-1.172634768D-02	2.228897169D-05								
-1.808702234D-08	5.421828530D-12		5.607264740D+04	-6.032261795D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15990.000
2.718212835D+05	-2.941949284D+03	1.559075626D+01	-8.093965740D-04	1.739434000D-07								
-1.932034262D-11	8.570339980D-16		6.274672550D+04	-6.207028885D+01								

C4 Gurvich, 1991 pt1 p18 pt2 p16.

3	g	tpis	C	4.00	0.00	0.00	0.00	0.00	0	48.0428000	1033903.742	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13117.742
3.903780500D+04	-8.948280780D+02	1.050952925D+01	-6.552894460D-03	1.243940464D-05								
-8.645341370D-09	2.263638846D-12		1.266425869D+05	-3.077594475D+01								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13117.742
9.200685130D+05	-1.530311800D+03	6.050069200D+00	5.252743670D-03	-1.779154772D-06								
2.589873632D-10	-1.385553481D-14		1.334389611D+05	-7.261148820D+00								
6000.000	20000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		13117.742
-2.864752103D+07	1.765535487D+04	6.166598280D+00	8.098789030D-04	-6.653483810D-08								
2.504726897D-12	-3.585724180D-17		-2.082319291D+04	4.331258920D+00								

C4H2, butadiyne 1,3-Butadiyne. Dorofeeva, 1991.

2	g	7/01	C	4.00H	2.00	0.00	0.00	0.00	0	50.0586800	450000.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		14393.860
2.467542569D+05	-3.897855640D+03	2.366080456D+01	-2.208077805D-02	2.781101140D-05								
-1.577340010D-08	3.423165460D-12		7.086907820D+04	-1.109173560D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		14393.860
2.328179913D+06	-8.925186090D+03	2.114326883D+01	-1.368871276D-03	2.327503159D-07								
-2.124517624D-11	8.053313020D-16		1.057788416D+05	-1.088313574D+02								

C4H4, 1,3-cyclo- 1,3-Cyclobutadiene. Dorofeeva, 1986.

2	g	8/00	C	4.00H	4.00	0.00	0.00	0.00	0	52.0745600	385000.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12103.534
-2.778428049D+04	1.768176915D+03	-1.757895171D+01	9.383512920D-02	-1.195524281D-04								
7.978086190D-08	-2.152751100D-11		3.811627120D+04	1.128478124D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		12103.534
2.991498949D+06	-1.416781502D+04	3.001978876D+01	-2.579200423D-03	4.789990450D-07								
-4.775329710D-11	1.974923662D-15		1.274666920D+05	-1.727532057D+02								

C4H6, butadiene 1,3-butadiene. TRC(10/92) tuvw2820.

2	n	10/92	C	4.00H	6.00	0.00	0.00	0.00	0	54.0904400	110000.000	
200.000	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15130.000
-9.181130530D+04	3.312570530D+03	-2.985828611D+01	1.479201147D-01	-2.056618326D-04								
1.466496826D-07	-4.145285730D-11		-2.077309444D+03	1.780687329D+02								
1000.000	6000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		15130.000
-2.361903188D+07	5.651323370D+04	-3.275738320D+01	2.293070572D-02	-2.297106441D-06								
4.292596210D-11	4.236766040D-15		-3.671358620D+05	3.013437302D+02								



## Appendix D (continued)

C4H6,1butyne TRC(10/93) tuv3040.

2 n10/93 C	4.00H	6.00	0.00	0.00	0.00	0.00	0	54.0904400	165200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.597039970D+04	1.433191711D+03	-9.691210720D+00	7.150002390D-02	-8.157967800D-05					
5.290364970D-08	-1.435655372D-11		1.184987013D+04	7.660225360D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.364402700D+06	-2.392087731D+04	4.073750410D+01	-3.176726490D-03	1.199856984D-07					
3.201802510D-11	-2.854392633D-15		1.634335546D+05	-2.460284791D+02					

C4H6,2butyne TRC(10/93) tuv3040.

2 n10/93 C	4.00H	6.00	0.00	0.00	0.00	0	54.0904400	145700.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.650756405D+05	4.490728690D+03	-2.400723889D+01	9.819579550D-02	-1.079717182D-04					
6.675555770D-08	-1.740766886D-11		-5.328363710D+03	1.595035268D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.981304330D+06	-1.873032899D+04	3.654561490D+01	-2.369686378D-03	3.990211810D-07					
-3.69870270D-11	1.442072006D-15		1.261460214D+05	-2.155866205D+02					

C4H6,cyclo- Cyclobutene. Dorofeeva,1986.

2 g 8/00 C	4.00H	6.00	0.00	0.00	0.00	0	54.0904400	156700.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.046707734D+05	4.919470570D+03	-3.753278160D+01	1.497293031D-01	-1.860139375D-04					
1.219909019D-07	-3.254073590D-11		-3.915950540D+03	2.233282138D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.517367820D+06	-2.097311985D+04	4.008039170D+01	-3.949793980D-03	7.448484990D-07					
-7.529754170D-11	3.153253502D-15		1.406469848D+05	-2.434836999D+02					

C4H8,1-butene TRC(4/88) tuv2600.

2 n 4/88 C	4.00H	8.00	0.00	0.00	0.00	0	56.1063200	-540.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.721492014D+05	5.100079250D+03	-3.183786250D+01	1.317754442D-01	-1.527359339D-04					
9.714761110D-08	-2.560204470D-11		-2.523096386D+04	2.006932108D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.257948610D+06	-2.660376305D+04	4.764920050D+01	-4.383267110D-03	7.128838440D-07					
-5.991020840D-11	2.051753504D-15		1.569252657D+05	-2.913869761D+02					

C4H8,cis2-buten Cis2-butene TRC(4/88) tuv2600.

2 n 4/88 C	4.00H	8.00	0.00	0.00	0.00	0	56.1063200	-7400.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.773870877D+05	5.382384040D+03	-3.375188100D+01	1.322980623D-01	-1.490975922D-04					
9.277722000D-08	-2.408282948D-11		-2.715884347D+04	2.114462085D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.461018350D+06	-2.775376432D+04	4.863532360D+01	-4.862386350D-03	8.412626100D-07					
-7.633890370D-11	2.861702826D-15		1.630856187D+05	-3.003105998D+02					

C4H8,tr2-butene TRC(4/88) tuv2600.

2 n 4/88 C	4.00H	8.00	0.00	0.00	0.00	0	56.1063200	-11000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.594644110D+05	5.930972080D+03	-3.255825290D+01	1.254957780D-01	-1.374705365D-04					
8.407341350D-08	-2.163047345D-11		-3.113296523D+04	2.070081219D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.444758090D+06	-2.750706151D+04	4.870329380D+01	-4.952445460D-03	8.700135910D-07					
-8.017471710D-11	3.052575093D-15		1.612137505D+05	-3.004419156D+02					

C4H8,isobutene TRC(4/88) tuv2600.

2 n 4/88 C	4.00H	8.00	0.00	0.00	0.00	0	56.1063200	-17100.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.327205032D+05	3.941994240D+03	-2.224581184D+01	1.012790864D-01	-1.073194065D-04					
6.454696910D-08	-1.646330345D-11		-2.233766063D+04	1.479597621D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.484970990D+06	-2.732504764D+04	4.836321080D+01	-4.768004050D-03	8.233875840D-07					
-7.449253000D-11	2.782303056D-15		1.595941773D+05	-2.982986237D+02					

C4H8,cyclo- Cyclobutane. Dorofeeva,1986.

2 g 8/00 C	4.00H	8.00	0.00	0.00	0.00	0	56.1063200	28400.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.047655983D+05	6.519482730D+03	-4.662987590D+01	1.743593052D-01	-2.090964176D-04					
1.343528679D-07	-3.542727400D-11		-2.700031171D+04	2.738348195D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.456213810D+06	-2.301018492D+04	4.492448460D+01	-3.080145176D-03	5.317165260D-07					
-5.081079380D-11	2.048919092D-15		1.355487603D+05	-2.771801965D+02					

## Appendix D (continued)

(CH<sub>3</sub>COOH)<sub>2</sub> Acetic acid dimer. Chao,1978.  
 2 g10/00 C 4.00H 8.00O 4.00 0.00 0.00 0 120.1039200 -929015.360  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28053.169  
 -3.094720023D+05 5.983338600D+03-3.573002920D+01 1.662525587D-01-1.883866300D-04  
 1.154939386D-07-2.935166753D-11 -1.421493469D+05 2.295855147D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28053.169  
 6.571327590D+06-3.036870720D+04 6.250376670D+01-5.732624710D-03 1.083461635D-06  
 -1.097963590D-10 4.609263380D-15 6.347426600D+04-3.734555070D+02

C<sub>4</sub>H<sub>9</sub>,n-butyl TRC(10/84) tuvwl940.  
 2 n10/84 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 66530.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19797.000  
 -2.239560407D+05 4.676554100D+03-2.985424449D+01 1.345493704D-01-1.600660350D-04  
 1.045338096D-07-2.812951048D-11 -1.525297704D+04 1.901651559D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19797.000  
 7.198686940D+06-2.959241524D+04 5.242042810D+01-5.441572440D-03 9.917758370D-07  
 -9.464455870D-11 3.729487040D-15 1.834566472D+05-3.214209170D+02

C<sub>4</sub>H<sub>9</sub>,i-butyl 2-methylpropyl. TRC(10/84) tuvwl940.  
 2 n10/84 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 57320.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18317.000  
 -2.399461281D+05 4.697444540D+03-3.087472560D+01 1.391655831D-01-1.670233968D-04  
 1.092423088D-07-2.936209962D-11 -1.638151036D+04 1.936662372D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18317.000  
 6.752936060D+06-2.837423721D+04 5.140687610D+01-4.982399010D-03 8.801506630D-07  
 -8.125738690D-11 3.099140009D-15 1.743448480D+05-3.149940745D+02

C<sub>4</sub>H<sub>9</sub>,s-butyl 1-methylpropyl radical. Tsang,1985.  
 2 g 1/93 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 71000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17537.649  
 -3.351062890D+05 6.312945950D+03-4.003025260D+01 1.563875047D-01-1.842331788D-04  
 1.182727848D-07-3.131156589D-11 -2.216045659D+04 2.481295714D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17537.649  
 7.224744350D+06-3.035291099D+04 5.288551830D+01-5.652083550D-03 1.060032692D-06  
 -1.066129835D-10 4.443810960D-15 1.883494279D+05-3.255719880D+02

C<sub>4</sub>H<sub>9</sub>,t-butyl 1,1dimethylethyl radical. Tsang,1985.  
 2 g 1/93 C 4.00H 9.00 0.00 0.00 0.00 0 57.1142600 51700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17009.675  
 -4.723461950D+05 6.090198770D+03-4.683675340D+01 1.575300095D-01-1.686559436D-04  
 9.981040130D-08-2.487608823D-11 -3.319367410D+04 2.894838706D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17009.675  
 7.151064950D+06-3.171224410D+04 5.442510320D+01-6.392331160D-03 1.241097612D-06  
 -1.287248300D-10 5.512618740D-15 1.934506997D+05-3.399325290D+02

C<sub>4</sub>H<sub>10</sub>,n-butane Hf:TRC(10/85) w1350. Chen,1975.  
 2 g12/00 C 4.00H 10.00 0.00 0.00 0.00 0 58.1222000 -125790.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19228.685  
 -3.175872540D+05 6.176331820D+03-3.891562120D+01 1.584654284D-01-1.860050159D-04  
 1.199676349D-07-3.201670550D-11 -4.540363390D+04 2.379488665D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19228.685  
 7.682322450D+06-3.256051510D+04 5.736732750D+01-6.197916810D-03 1.180186048D-06  
 -1.221893698D-10 5.250635250D-15 1.774526560D+05-3.587918760D+02

C<sub>4</sub>H<sub>10</sub>,isobutane TRC(10/85) w1350. Chen,1975.  
 2 g 8/00 C 4.00H 10.00 0.00 0.00 0.00 0 58.1222000 -134990.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17936.500  
 -3.834469330D+05 7.000039640D+03-4.440026900D+01 1.746183447D-01-2.078195348D-04  
 1.339792433D-07-3.551681630D-11 -5.034018890D+04 2.658966497D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17936.500  
 7.528018920D+06-3.202517060D+04 5.700161000D+01-6.060013090D-03 1.143975809D-06  
 -1.157061835D-10 4.846042910D-15 1.728500802D+05-3.576176890D+02

C<sub>4</sub>N<sub>2</sub> Hf:TRC(12/93) w8992. Khanna,1987. Brown,1989.  
 2 g 6/01 C 4.00N 2.00 0.00 0.00 0.00 0 76.0562000 529200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17799.401  
 1.587802866D+05-2.987184206D+03 2.348081602D+01-2.607502448D-02 4.042830030D-05  
 -2.804912444D-08 7.397652050D-12 7.505299470D+04-1.017578250D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17799.401  
 1.167686152D+06-6.198644180D+03 2.062070093D+01-1.518619449D-03 3.162361680D-07  
 -3.469922800D-11 1.555154128D-15 9.667409390D+04-9.669734738D+01

## Appendix D (continued)

C5 Gurvich,1991 pt1 p20 pt2 p18.

3 g 8/00 C	5.00	0.00	0.00	0.00	0.00	0.00	0.00	60.0535000	1050924.332
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.200801119D+04	-5.553702910D+02	1.123828271D+01	-4.347884520D-03	1.738987490D-05					
-1.707945418D-08	5.574541910D-12		1.262404627D+05	-3.262308990D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.172055356D+05	-2.958510027D+03	1.561080967D+01	-8.200361920D-04	1.776898025D-07					
-2.009853583D-11	9.222677770D-16		1.395208064D+05	-6.433077180D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.266863960D+06	-2.666377675D+03	1.408383780D+01	-6.620512140D-05	4.099789450D-09					
-1.315689998D-13	1.711940703D-18		1.405413771D+05	-5.349354010D+01					
C5H6,1,3cyclo-	1,3-Cyclopentadiene. Pedley,1986	p90.	Dorofeeva,1986.						
2 g 5/90 C	5.00H	6.00	0.00	0.00	0.00	0	66.1011400	134300.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.886259728D+05	4.738220870D+03	-3.888958010D+01	1.667438533D-01	-2.141149581D-04					
1.438132328D-07	-3.906478110D-11		-5.667022010D+03	2.279898557D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.428478190D+06	-2.123547976D+04	4.309819010D+01	-3.914783460D-03	7.311847010D-07					
-7.327241190D-11	3.044403403D-15		1.382542782D+05	-2.605959678D+02					
C5H8,cyclo-	Cyclopentene. Hf:TRC(10/92)	w2840.	Dorofeeva,1986.						
2 g 1/93 C	5.00H	8.00	0.00	0.00	0.00	0	68.1170200	33900.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.631114588D+05	5.987753490D+03	-4.522244600D+01	1.804626339D-01	-2.177216062D-04					
1.402022671D-07	-3.699094300D-11		-2.379504749D+04	2.660136401D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.569848100D+06	-2.406018294D+04	4.881006460D+01	-3.413054980D-03	6.047001660D-07					
-5.927495780D-11	2.447865390D-15		1.413983093D+05	-2.989533527D+02					
C5H10,1-pentene	TRC(4/87)	tuwv2500.							
2 n 4/87 C	5.00H	10.00	0.00	0.00	0.00	0	70.1329000	-21280.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.340548130D+05	9.298917380D+03	-5.667792450D+01	2.123100266D-01	-2.571298290D-04					
1.666834304D-07	-4.434080470D-11		-4.790682180D+04	3.396036400D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.744014970D+06	-2.104485321D+04	4.736126990D+01	-4.244201200D-04	-3.898975050D-08					
1.367074243D-11	-9.313194230D-16		1.154091373D+05	-2.786177449D+02					
C5H10,cyclo-	Cyclopentane. Dorofeeva,1986.								
2 g 2/01 C	5.00H	10.00	0.00	0.00	0.00	0	70.1329000	-77100.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.141119710D+05	8.627592800D+03	-6.202959980D+01	2.259910921D-01	-2.682303330D-04					
1.706289935D-07	-4.464050920D-11		-4.931522140D+04	3.583916230D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.501938730D+06	-3.505864850D+04	6.322480750D+01	-6.940356580D-03	1.337306593D-06					
-1.377905033D-10	5.867357640D-15		1.954925511D+05	-4.026550900D+02					
C5H11,pentyl	Radical. TRC(10/84)	tuwv1941.							
2 n10/84 C	5.00H	11.00	0.00	0.00	0.00	0	71.1408400	45810.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.653715920D+05	8.564220420D+03	-5.295242890D+01	2.094288859D-01	-2.561602906D-04					
1.692755961D-07	-4.596788110D-11		-3.641704270D+04	3.196862240D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.697252900D+06	-2.891706175D+04	5.811029680D+01	-3.593995010D-03	4.419967630D-07					
-1.509664551D-11	-6.626964430D-16		1.717009550D+05	-3.522477120D+02					
C5H11,t-pentyl	1,1-dimethylpropyl radical. Tsang,1985.								
2 g 1/93 C	5.00H	11.00	0.00	0.00	0.00	0	71.1408400	32600.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.152181980D+05	9.144327830D+03	-5.602397890D+01	1.998204194D-01	-2.239112591D-04					
1.375455547D-07	-3.523833050D-11		-4.036266610D+04	3.402811000D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.602108260D+06	-3.805205770D+04	6.649690370D+01	-7.533860630D-03	1.451612787D-06					
-1.495593207D-10	6.368022330D-15		2.281858805D+05	-4.169408550D+02					
C5H12,n-pentane	TRC(10/85)	tuwv1350.							
2 n10/85 C	5.00H	12.00	0.00	0.00	0.00	0	72.1487800	-146760.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.768894625D+05	5.834283470D+03	-3.617541480D+01	1.533339707D-01	-1.528395882D-04					
8.191092000D-08	-1.792327902D-11		-4.665375250D+04	2.265544053D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.530779286D+06	-8.972593260D+03	4.536223260D+01	-2.626989916D-03	3.135136419D-06					
-5.318728940D-10	2.886896868D-14		1.484616529D+04	-2.516550384D+02					

## Appendix D (continued)

C5H12,i-pentane 2-Methylbutane. TRC(10/85) tuvwl350.

2 n10/85 C	5.00H	12.00	0.00	0.00	0.00	0.00	0	72.1487800	-153700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.231903390D+05	6.497189100D+03	-3.681126970D+01	1.532424729D-01	-1.548790714D-04					
8.749897120D-08	-2.070547710D-11		-5.155416590D+04	2.309518218D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.156888594D+07	-4.556246870D+04	7.495443630D+01	-7.845415580D-03	1.444393314D-06					
-1.464370213D-10	6.230285000D-15		2.544927135D+05	-4.801985780D+02					

CH3C(CH3)2CH3 2,2-Dimethylpropane (neopentane). TRC(10/85) tuvwl350.

2 n10/85 C	5.00H	12.00	0.00	0.00	0.00	0.00	0	72.1487800	-167920.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.97322270D+06	1.289225617D+05	-7.199344830D+02	2.056862183D+00	-2.953159699D-03					
2.158893146D-06	-6.268318770D-10		-6.394932020D+05	4.020806360D+03					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.684705520D+07	-5.979430570D+04	8.685451480D+01	-9.621917600D-03	1.653363091D-06					
-1.674727926D-10	7.372119360D-15		3.458496820D+05	-5.760466970D+02					

C6D5,phenyl Radical-d5. Burcat,1985.

2 g 1/01 C	6.00D	5.00	0.00	0.00	0.00	0.00	0	82.1347100	315740.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.012837008D+05	-1.979349332D+03	2.628267500D+00	5.951865260D-02	-6.081280450D-05					
3.381391650D-08	-8.125429080D-12		4.697247490D+04	3.354700980D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.411628125D+06	-1.362569472D+04	4.028984940D+01	-3.490989270D-03	7.379612130D-07					
-8.192244050D-11	3.705330970D-15		1.088073731D+05	-2.293621057D+02					

C6D6 Benzene-d6. Burcat,1985.

2 g 1/01 C	6.00D	6.00	0.00	0.00	0.00	0.00	0	84.1488120	58157.378
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.762911236D+05	-2.865868902D+03	5.395070430D+00	5.939315170D-02	-6.023631180D-05					
3.381398570D-08	-8.306046370D-12		2.047083778D+04	-2.011790696D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.758057871D+06	-1.572121558D+04	4.468162490D+01	-4.003361920D-03	8.445434400D-07					
-9.360556980D-11	4.228475530D-15		8.962045360D+04	-2.615332268D+02					

C6H2 Dorofeeva,1991.

2 g 2/93 C	6.00H	2.00	0.00	0.00	0.00	0.00	0	74.0800800	670000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.903722964D+05	-4.929751500D+03	3.189323210D+01	-3.119447315D-02	4.325763680D-05					
-2.732517022D-08	6.674446110D-12		1.011898682D+05	-1.530593012D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.592848577D+06	-1.083361978D+04	2.847459495D+01	-1.876727704D-03	3.412134280D-07					
-3.337392890D-11	1.356853889D-15		1.418517294D+05	-1.494853494D+02					

C6H5,phenyl Radical.Hf:TRC(10/89) w4270. Jacox,1989. NASA ab initio.

2 g11/00 C	6.00H	5.00	0.00	0.00	0.00	0.00	0	77.1039000	337200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.211278245D+05	3.529045580D+03	-3.116903422D+01	1.467550630D-01	-1.831398296D-04					
1.192576957D-07	-3.149265860D-11		2.420972928D+04	1.868799946D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.670279230D+06	-1.894601209D+04	4.180581820D+01	-3.503914150D-03	6.561821740D-07					
-6.594714450D-11	2.748094212D-15		1.476744628D+05	-2.475301142D+02					

C6H5O,phenoxy Phenoxy radical. Burcat,1985.

2 g 8/00 C	6.00H	5.00O	1.00	0.00	0.00	0.00	0	93.1033000	47700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.292264217D+05	3.406740680D+03	-2.911367361D+01	1.459180378D-01	-1.780202758D-04					
1.138615885D-07	-2.967142152D-11		-1.055026758D+04	1.770682011D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.678640340D+06	-1.972980806D+04	4.541184410D+01	-3.751064390D-03	7.114450780D-07					
-7.233328850D-11	3.045637067D-15		1.163595961D+05	-2.681058539D+02					

C6H6 TRC(10/86) w3200. Pliva,1982,1983,1984. Shimanouchi,1972.

2 g 8/00 C	6.00H	6.00	0.00	0.00	0.00	0.00	0	78.1118400	82880.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.677340902D+05	4.404500040D+03	-3.717377910D+01	1.640509559D-01	-2.020812374D-04					
1.307915264D-07	-3.444284100D-11		-1.035455401D+04	2.169853345D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.538575720D+06	-2.260502547D+04	4.694007300D+01	-4.206676830D-03	7.907994330D-07					
-7.968302100D-11	3.328212080D-15		1.391464686D+05	-2.868751333D+02					

## Appendix D (continued)

C6H5OH, phenol      Burcat, 1985.  
 2 g 8/00 C    6.00H    6.00O    1.00    0.00    0.00 0    94.1112400    -96399.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17496.700  
 -1.209418144D+05 3.378292270D+03-2.991846148D+01 1.567802942D-01-1.970937198D-04  
 1.291815064D-07-3.424351260D-11    -2.779387017D+04 1.799708977D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17496.700  
 4.462081570D+06-2.165521026D+04 4.815015050D+01-3.568282430D-03 6.327175730D-07  
 -6.039905720D-11 2.399168678D-15    1.113726204D+05-2.860454446D+02

C6H10, cyclo-      Cyclohexene. Dorofeeva, 1986.  
 2 g 1/93 C    6.00H    10.00    0.00    0.00    0.00 0    82.1436000    -4600.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17270.784  
 -3.750282210D+05 7.643876750D+03-5.510434760D+01 2.166231405D-01-2.545452198D-04  
 1.607607304D-07-4.185248410D-11    -3.661073010D+04 3.202409460D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17270.784  
 7.510128980D+06-3.556858210D+04 6.703034940D+01-7.045351870D-03 1.358166400D-06  
 -1.400074492D-10 5.964551700D-15    2.060274332D+05-4.238197660D+02

C6H12, 1-hexene      TRC(4/87) tuv2500.  
 2 n 4/87 C    6.00H    12.00    0.00    0.00    0.00 0    84.1594800    -41950.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    26240.000  
 -6.668831650D+05 1.176864939D+04-7.270998330D+01 2.709398396D-01-3.333246400D-04  
 2.182347097D-07-5.859468820D-11    -6.215780540D+04 4.286825640D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    26240.000  
 7.332906960D+05-1.448848641D+04 4.671215490D+01 3.172978470D-03-5.242646520D-07  
 4.280355820D-11-1.472353254D-15    6.697740410D+04-2.623643854D+02

C6H12, cyclo-      Cyclohexane. Dorofeeva, 1986.  
 2 g 6/90 C    6.00H    12.00    0.00    0.00    0.00 0    84.1594800    -123300.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17544.814  
 -5.679987040D+05 1.034238704D+04-6.800041250D+01 2.387797658D-01-2.511890049D-04  
 1.425293184D-07-3.407833190D-11    -6.404635160D+04 3.934808210D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17544.814  
 5.225149470D+06-3.364194580D+04 7.174607470D+01-6.698979120D-03 1.318443254D-06  
 -1.390794789D-11-1.472353254D-15    1.732537609D+05-4.546814170D+02

C6H13, n-hexyl      TRC(10/83) tuv1930.  
 2 n10/83 C    6.00H    13.00    0.00    0.00    0.00 0    85.1674200    25100.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    28983.000  
 -1.427278220D+06 2.248828093D+04-1.297492240D+02 4.279797330D-01-5.556013180D-04  
 3.791256940D-07-1.048462404D-10    -1.060261015D+05 7.497186760D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    28983.000  
 5.967938620D+06-3.299023160D+04 6.869073440D+01-4.225009060D-03 5.496523820D-07  
 -2.292851471D-11-5.086341890D-16    1.906978683D+05-4.185362000D+02

C6H14, n-hexane      TRC(4/85) tuv1440.  
 2 g 6/01 C    6.00H    14.00    0.00    0.00    0.00 0    86.1753600    -166920.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    28702.000  
 -5.815926700D+05 1.079097724D+04-6.633947030D+01 2.523715155D-01-2.904344705D-04  
 1.802201514D-07-4.617223680D-11    -7.271544570D+04 3.938283540D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    28702.000  
 -3.106625684D+06-7.346087920D+03 4.694131760D+01 1.693963977D-03 2.068996667D-06  
 -4.212141680D-10 2.452345845D-14    5.237503120D+02-2.549967718D+02

C7H7, benzyl      Radical. Brouwer, 1988. Hippler, 1990.  
 2 g 7/01 C    7.00H    7.00    0.00    0.00    0.00 0    91.1304800    210500.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18554.892  
 -1.836764826D+05 4.102465660D+03-3.202406100D+01 1.588249575D-01-1.894466924D-04  
 1.203649671D-07-3.136589637D-11    5.266333230D+03 1.938751720D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18554.892  
 5.297322160D+06-2.599909398D+04 5.509750790D+01-4.977661470D-03 9.463152430D-07  
 -9.639008860D-11 4.064470420D-15    1.738382912D+05-3.343829550D+02

C7H8      Hf:TRC(4/98) w3510. Hitchcock, 1975. Rudolph, 1967.  
 2 g 1/93 C    7.00H    8.00    0.00    0.00    0.00 0    92.1384200    50170.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17940.345  
 -2.877962220D+05 6.133941520D+03-4.574706760D+01 1.936895724D-01-2.304305304D-04  
 1.459301178D-07-3.790796100D-11    -2.308402499D+04 2.693915042D+02  
 1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17940.345  
 6.184538350D+06-2.990284056D+04 5.982005970D+01-5.696983960D-03 1.080748416D-06  
 -1.098702235D-10 4.624740220D-15    1.782047857D+05-3.698082250D+02

## Appendix D (continued)

C7H8O,cresol-mx Eql. mixture of isomers. Kudchadker,1978.

2 g12/00 C	7.00H	8.000	1.00	0.00	0.00	0	108.1378200	-132298.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.441417503D+05	5.080877840D+03	-3.789048040D+01	1.864945070D-01	-2.269511868D-04				
1.458989279D-07	-3.822403350D-11		-4.093657830D+04	2.281352234D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.017373450D+06	-2.849882774D+04	6.081543070D+01	-4.996807110D-03	9.134279950D-07				
-8.979444110D-11	3.667756970D-15		1.472218400D+05	-3.674850140D+02				

C7H14,1-heptene TRC(4/87) tuv2500.

2 n 4/87 C	7.00H	14.00	0.00	0.00	0.00	0	98.1860600	-62760.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.449402840D+05	1.332179893D+04	-8.281694380D+01	3.108065994D-01	-3.786779920D-04				
2.446841042D-07	-6.488763870D-11		-7.217885010D+04	4.856671490D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.927608174D+06	-9.125024420D+03	4.748177970D+01	6.067660530D-03	-8.684859080D-07				
5.813995260D-11	-1.473979569D-15		2.600914656D+04	-2.562880707D+02				

C7H15,n-heptyl TRC(10/83) tuv1930.

2 n10/83 C	7.00H	15.00	0.00	0.00	0.00	0	99.1940000	4390.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.671733521D+06	2.640010250D+04	-1.526867707D+02	5.027121410D-01	-6.521014030D-04				
4.443488110D-07	-1.227815006D-10		-1.273754623D+05	8.783933320D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.444527570D+06	-3.456829290D+04	7.638651950D+01	-3.298972000D-03	2.343496957D-07				
2.467674021D-11	-3.162012849D-15		1.939079354D+05	-4.641424660D+02				

C7H16,n-heptane TRC(10/85) tuv1460. TRC(10/84) ptuv1010.

2 n10/85 C	7.00H	16.00	0.00	0.00	0.00	0	100.2019400	-187780.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.127432890D+05	1.184085437D+04	-7.487188600D+01	2.918466052D-01	-3.416795490D-04				
2.159285269D-07	-5.655852730D-11		-8.013408940D+04	4.407213320D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.135632470D+06	-3.923319690D+04	7.889780850D+01	-4.654251930D-03	2.071774142D-06				
-3.442539300D-10	1.976834775D-14		2.050708295D+05	-4.851104020D+02				

C7H16,2-methylh 2-methylhexane. TRC(10/85) tuv1460.

2 n10/85 C	7.00H	16.00	0.00	0.00	0.00	0	100.2019400	-194600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.10477770D+05	1.191251120D+04	-7.345339440D+01	2.902952369D-01	-3.462767680D-04				
2.260184498D-07	-6.128813920D-11		-8.202147700D+04	4.320042290D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.289912969D+06	-1.784340963D+03	1.083537673D+01	5.270609240D-02	-1.886832314D-05				
2.432255843D-09	-1.13553789D-13		-1.637529884D+04	-2.981862410D+01				

C8H8,styrene Ethenylbenzene. TRC(4/89) tuv4490.

2 n 4/89 C	8.00H	8.00	0.00	0.00	0.00	0	104.1491200	148300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.686930520D+05	6.167999470D+03	-4.836054940D+01	2.182873229D-01	-2.738561832D-04				
1.810084981D-07	-4.867750270D-11		-1.140639978D+04	2.817679014D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.629183620D+06	1.514594166D+04	1.609822364D+00	3.383318600D-02	-1.093737395D-05				
1.338825116D-09	-6.032534920D-14		-8.997324150D+04	4.311282790D+01				

C8H10,ethylbenz Ethylbenzene. TRC(10/86) tuv3200.

2 n10/86 C	8.00H	10.00	0.00	0.00	0.00	0	106.1650000	29920.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.694940000D+05	9.307168360D+03	-6.521769470D+01	2.612080237D-01	-3.181753480D-04				
2.051355473D-07	-5.401817350D-11		-4.073870210D+04	3.780904360D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.551564100D+06	-2.831380598D+04	6.061240720D+01	1.042112857D-03	-1.327426719D-06				
2.166031743D-10	-1.142545514D-14		1.642241062D+05	-3.691769820D+02				

C8H16,1-octene TRC(4/87) tuv2500.

2 n 4/87 C	8.00H	16.00	0.00	0.00	0.00	0	112.2126400	-83590.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.281905220D+05	1.640974476D+04	-1.015939534D+02	3.748001410D-01	-4.590829400D-04				
2.965335340D-07	-7.840445210D-11		-8.952426080D+04	5.907594270D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.409336070D+06	-4.383678800D+03	4.939154260D+01	7.912339630D-03	-7.888669510D-07				
9.970212350D-12	1.913144872D-15		-1.122619342D+04	-2.577650649D+02				

## Appendix D (continued)

C8H17,n-octyl TRC(10/83) tuvwl930.  
 2 n10/83 C 8.00H 17.00 0.00 0.00 0.00 0 113.2205800 -16320.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38103.000  
 -1.934340995D+06 3.054979830D+04-1.767903454D+02 5.801596650D-01-7.517414010D-04  
 5.112469030D-07-1.410193662D-10 -1.498894706D+05 1.013724329D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38103.000  
 5.632173390D+06-3.821143670D+04 8.637927500D+01-3.608931580D-03 2.544260445D-07  
 2.908638837D-11-3.679549740D-15 2.103135470D+05-5.262422830D+02

C8H18,n-octane TRC(4/85) tuvwl490.  
 2 n 4/85 C 8.00H 18.00 0.00 0.00 0.00 0 114.2285200 -208750.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 37780.000  
 -6.986647150D+05 1.338501096D+04-8.415165920D+01 3.271936660D-01-3.777209590D-04  
 2.339836988D-07-6.010892650D-11 -9.026223250D+04 4.939222140D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 37780.000  
 6.365406950D+06-3.105364657D+04 6.969162340D+01 1.048059637D-02-4.129621950D-06  
 5.543226320D-10-3.819190110D-14 1.500968785D+05-4.169895650D+02

C8H18,isooctane 2,2,4-Trimethylpentane. TRC(4/85) tuvwl490.  
 2 n 4/85 C 8.00H 18.00 0.00 0.00 0.00 0 114.2285200 -224010.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32170.000  
 -1.688758565D+05 3.126903227D+03-2.123502828D+01 1.489151508D-01-1.151180135D-04  
 4.473216170D-08-5.554882070D-12 -4.468060620D+04 1.417455793D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32170.000  
 1.352765032D+07-4.663370340D+04 7.795313180D+01 1.423729984D-02-5.073593910D-06  
 7.248232970D-11-3.819190110D-14 2.541178017D+05-4.933887190D+02

C9H19,n-nonyl TRC (10/83) tuvwl930.  
 2 n10/83 C 9.00H 19.00 0.00 0.00 0.00 0 127.2471600 -37030.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 42664.000  
 -2.194880612D+06 3.468565780D+04-2.009261419D+02 6.580503110D-01-8.525930010D-04  
 5.794638960D-07-1.597637099D-10 -1.723194608D+05 1.149114017D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 42664.000  
 5.277361740D+06-4.025701960D+04 9.457296720D+01-2.940301447D-03 6.978106990D-09  
 6.805250240D-11-5.907095330D-15 2.165320614D+05-5.754449500D+02

C10H8,naphthalene Naphthalene. Chen,1979.  
 2 g 3/01 C 10.00H 8.00 0.00 0.00 0.00 0 128.1705200 150580.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20713.076  
 -2.602845316D+06 3.237409570D+04-5.226095040D+01 2.397692776D-01-2.912244803D-04  
 1.854944401D-07-4.816619270D-11 -1.114700880D+04 2.972139517D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20713.076  
 5.906172110D+06-3.163229240D+04 7.030342030D+01-6.018865540D-03 1.142052144D-06  
 -1.161605689D-10 4.892844020D-15 1.962567046D+05-4.347848950D+02

C10H21,n-decyl TRC(10/83) tuvwl930.  
 2 n10/83 C 10.00H 21.00 0.00 0.00 0.00 0 141.2737400 -57740.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 47224.000  
 -2.446511152D+06 3.870081300D+04-2.244388176D+02 7.343624970D-01-9.513525600D-04  
 6.462970330D-07-1.781502862D-10 -1.941633889D+05 1.280987834D+03  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 47224.000  
 4.967237760D+06-4.242468440D+04 1.028853417D+02-2.324848180D-03-2.284233900D-07  
 1.056127364D-10-8.068065900D-15 2.235429890D+05-6.255191160D+02

C12H9,o-bipheny o-Biphenyl radical. Burcat,1985.  
 2 g 8/00 C 12.00H 9.00 0.00 0.00 0.00 0 153.1998600 427730.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26589.347  
 -3.595840820D+05 7.661378560D+03-5.873290460D+01 2.697557882D-01-3.229756680D-04  
 2.032907100D-07-5.231316720D-11 1.458414642D+04 3.392687110D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26589.347  
 6.736469420D+06-3.632194350D+04 8.210239600D+01-7.502342860D-03 1.456251733D-06  
 -1.507145019D-10 6.436470430D-15 2.555524521D+05-5.042462970D+02

C12H10,biphenyl Burcat,1985.  
 2 g 8/00 C 12.00H 10.00 0.00 0.00 0.00 0 154.2078000 182130.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26783.523  
 -3.671034050D+05 8.128412590D+03-6.390994570D+01 2.901422744D-01-3.509590740D-04  
 2.230989996D-07-5.788470290D-11 -1.679263066D+04 3.633464190D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26783.523  
 7.480385360D+06-3.928087230D+04 8.661482220D+01-7.946398570D-03 1.531868544D-06  
 -1.576450171D-10 6.700602730D-15 2.438050641D+05-5.381381490D+02

## Appendix D (continued)

Ca Hf:Cox,1989. Sugar,1985. Gordon,1999.

3 g 8/97 CA	1.00	0.00	0.00	0.00	0.00	0.00	0	40.0780000	177800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							2.063892786D+04	4.384548330D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.547341240D+06	-2.148642662D+04	2.530849567D+01	-1.103773705D-02	2.293249636D-06					
-1.209075383D-10	-4.015333268D-15			1.585862323D+05	-1.609512955D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.291781634D+09	-1.608862960D+06	4.312466360D+02	-5.396508990D-02	3.531856210D-06					
-1.164403850D-10	1.527134223D-15			1.258651434D+07	-3.692101610D+03				

Ca+ Sugar,1985. Gordon,1999.

3 g 1/98 CA	1.00E	-1.00	0.00	0.00	0.00	0	40.0774514	773827.728	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							9.232417790D+04	5.077674980D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.747070820D+06	-1.174707738D+04	1.672546969D+01	-8.334797710D-03	2.394593294D-06					
-2.988243468D-10	1.356563002D-14			1.664329088D+05	-9.582821260D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.117128410D+08	-6.220428460D+05	1.683741136D+02	-2.140862670D-02	1.452947686D-06					
-4.920790880D-11	6.575369235D-16			4.959472060D+06	-1.422600719D+03				

CaBr Gurvich,1996a pt1 p471 pt2 p367.

2 tpis96 CA	1.00BR	1.00	0.00	0.00	0.00	0	119.9820000	-24868.681	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.693832620D+02	-1.257513537D+02	5.001508330D+00	-1.039868753D-03	1.377594927D-06					
-8.949013960D-10	2.395658928D-13			-3.728103980D+03	1.784864847D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.783236402D+06	-8.458203730D+03	1.431756560D+01	-5.430781680D-03	1.522218659D-06					
-1.831824807D-10	7.864288660D-15			4.931270680D+04	-6.537001100D+01				

CaBr2 Gurvich,1996a pt1 p474 pt2 p369.

2 tpis96 CA	1.00BR	2.00	0.00	0.00	0.00	0	199.8860000	-387197.300	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.572504318D+03	-2.238551236D+02	8.388457890D+00	-1.944164774D-03	2.397926088D-06					
-1.556572350D-09	4.124309580D-13			-4.772106610D+04	-1.074965233D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.219846426D+04	-4.463155330D+00	7.503755110D+00	-1.641654626D-06	3.879428060D-10					
-4.683424260D-14	2.259325541D-18			-4.885436820D+04	-5.590324250D+00				

CaCL Gurvich,1996a pt1 p464 pt2 p363.

2 tpis96 CA	1.00CL	1.00	0.00	0.00	0.00	0	75.5310000	-103772.885	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.395335260D+03	-2.249042269D+02	5.283278390D+00	-1.447983237D-03	1.643742771D-06					
-9.430104280D-10	2.237516133D-13			-1.270169000D+04	-1.391964289D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.629182545D+06	-4.766223020D+03	9.658929770D+00	-2.523044131D-03	5.833542160D-07					
-4.101726990D-11	8.813177640D-17			1.662599241D+04	-3.398731174D+01				

CaCL+ Gurvich,1996a pt1 p466 pt2 p364.

2 tpis96 CA	1.00CL	1.00E	-1.00	0.00	0.00	0	75.5304514	467190.513	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.285284542D+03	-2.002872721D+02	4.936990190D+00	-3.860973030D-04	8.686661880D-08					
1.470205680D-10	-7.689315870D-14			5.588277950D+04	-6.359815341D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.770280396D+05	-5.891372390D+02	5.103368800D+00	-2.356761168D-04	5.483732870D-08					
2.137973112D-14	-5.572887310D-16			5.853417250D+04	-2.191253644D+00				

CaCL2 Gurvich,1996a pt1 p470 pt2 p366.

2 tpis96 CA	1.00CL	2.00	0.00	0.00	0.00	0	110.9840000	-485243.477	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.106802030D+04	-4.249108250D+02	9.134711860D+00	-3.497185310D-03	4.242184630D-06					
-2.719673231D-09	7.138268630D-13			-5.850346760D+04	-1.808678294D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.595768780D+04	-8.796495630D+00	7.507256910D+00	-3.129465934D-06	7.322886480D-10					
-8.776403220D-14	4.210486040D-18			-6.066779660D+04	-8.553523451D+00				

CaF Gurvich,1996a pt1 p456 pt2 p359.

2 tpis96 CA	1.00F	1.00	0.00	0.00	0.00	0	59.0764032	-276403.790	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.184235400D+04	-4.918235090D+02	5.701120890D+00	-1.465138218D-03	9.092930810D-07					
-1.367585222D-10	-5.106323380D-14			-3.197694110D+04	-5.996662260D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.195882670D+05	-1.512321567D+03	5.869276250D+00	-3.882524480D-04	-2.484582298D-08					
3.749915960D-11	-3.470976450D-15			-2.488814584D+04	-8.614663700D+00				



## Appendix D (continued)

CaF+ Gurvich,1996a pt1 p460 pt2 p360.  
 2 tps96 CA 1.00F 1.00E -1.00 0.00 0.00 0 59.0758546 260664.608  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9003.108  
 4.158340800D+04-5.627661660D+02 5.687522150D+00-1.264710572D-03 6.669086480D-07  
 -6.926752820D-11-3.978714620D-14 3.305119500D+04-6.974485010D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9003.108  
 -1.398670845D+05 2.191526375D+02 4.214324340D+00 2.142798048D-04-5.778672600D-08  
 9.985756310D-12-6.059621880D-16 2.841605897D+04 2.740342729D+00

CaF2 Gurvich,1996a pt1 p462 pt2 p362.  
 2 tps96 CA 1.00F 2.00 0.00 0.00 0.00 0 78.0748064 -790828.409  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12811.591  
 5.909352290D+04-1.019733042D+03 1.013165309D+01-5.503506440D-03 5.629319980D-06  
 -3.115401465D-09 7.205525940D-13 -9.192608190D+04-2.639505950D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12811.591  
 -8.280409440D+04-3.115950071D+01 7.023577370D+00-9.521000020D-06 2.118160895D-09  
 -2.440713888D-13 1.135135468D-17 -9.729466770D+04-7.546243340D+00

CaH Gurvich,1996a pt1 p447 pt2 p353.  
 2 tps96 CA 1.00H 1.00 0.00 0.00 0.00 0 41.0859400 229409.105  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8705.105  
 -4.513782230D+04 7.629429210D+02-1.280874223D+00 1.318774659D-02-1.481595334D-05  
 8.536573220D-09-1.989958945D-12 2.300378814D+04 3.053421525D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8705.105  
 -2.696952529D+06 8.607059750D+03-7.027454820D+00 7.467916310D-03-2.318610699D-06  
 3.423072420D-10-1.892679792D-14 -2.773819107D+04 7.845822010D+01

CaI Gurvich,1996a pt1 p474 pt2 p370.  
 2 tps96 CA 1.00I 1.00 0.00 0.00 0.00 0 166.9824700 12183.320  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.120  
 -8.261790180D+03-1.459821761D+02 4.864171690D+00-7.863169650D-04 1.100493506D-06  
 -7.348030610D-10 2.010892767D-13 5.236753440D+02 3.585391680D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.120  
 1.771071309D+06-5.683643730D+03 1.153857476D+01-4.194020200D-03 1.291359961D-06  
 -1.730043579D-10 8.380762350D-15 3.583293200D+04-4.405917570D+01

CaI2 Gurvich,1996a pt1 p477 pt2 p372.  
 2 tps96 CA 1.00I 2.00 0.00 0.00 0.00 0 293.8869400 -259319.505  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16050.995  
 -1.097851401D+03-1.459821761D+02 8.089341840D+00-1.305332923D-03 1.624199331D-06  
 -1.061194001D-09 2.825551217D-13 -3.272692980D+04-6.981714940D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16050.995  
 -1.623727104D+04-2.859530722D+00 7.502432190D+00-1.071178707D-06 2.544559095D-10  
 -3.083631004D-14 1.491836724D-18 -3.346341170D+04-3.567305740D+00

CaO Gurvich,1996a pt1 p443 pt2 p349.  
 3 tps96 CA 1.00O 1.00 0.00 0.00 0.00 0 56.0774000 38005.308  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8953.108  
 3.889733070D+04-4.835677350D+02 5.077713250D+00 3.076235250D-04-1.159759897D-06  
 8.493433340D-10-1.495333366D-13 5.937643480D+03-3.955320730D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8953.108  
 -4.913106170D+07 1.495865950D+05-1.681654149D+02 9.381950260D-02-2.455529428D-05  
 3.074980720D-09 1.485914237D-13 -9.461511720D+05 1.235694769D+03  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8953.108  
 -3.504055130D+08 2.083212387D+05-3.978209270D+01 5.039268720D-03-3.220707680D-07  
 1.057379426D-11-1.396044154D-16 -1.662378721D+06 3.934491930D+02

CaO+ Gurvich,1996a pt1 p445 pt2 p351.  
 3 tps96 CA 1.00O 1.00E -1.00 0.00 0.00 0 56.0768514 710237.542  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9163.110  
 1.098060332D+05-1.459992448D+03 9.880777940D+00-9.157564600D-03 8.707582560D-06  
 -4.390411080D-09 9.264854660D-13 9.150057350D+04-3.009947701D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9163.110  
 9.397843130D+05-2.993362243D+03 8.336191820D+00-2.303295087D-03 7.373967530D-07  
 -1.052888279D-10 5.257138410D-15 1.028098401D+05-2.461547836D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9163.110  
 -7.648645260D+07 1.739245253D+04 8.420288710D+00-1.168386844D-03 8.413684900D-08  
 -2.770799280D-12 3.569474430D-17 -8.643489770D+04-2.376513061D+01

CaOH Gurvich,1996a pt1 p451 pt2 p355.  
 2 tps96 CA 1.00O 1.00H 1.00 0.00 0.00 0 57.0853400 -173307.350  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11049.697  
 4.620028900D+04-9.285672820D+02 9.175828770D+00-3.962828800D-03 2.505447308D-06  
 3.852068210D-11-3.352778470D-13 -1.798009717D+04-2.533704850D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11049.697  
 1.979972994D+06-5.598880990D+03 1.151348706D+01-1.668264707D-03 3.312573910D-07  
 -1.789056647D-11-3.580716410D-16 1.340196822D+04-4.646084260D+01

## Appendix D (continued)

CaOH+ Gurvich,1996a pt1 p452 pt2 p356.

2 tpris96 CA	1.000	1.00H	1.00E	-1.00	0.00	0	57.0847914	372938.100
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.884342660D+04	-9.832415100D+02	9.610182950D+00	-5.204360660D-03	4.263049820D-06				
-1.197590878D-09	9.028411890D-15		4.795056340D+04	-2.827077334D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.637615370D+05	-2.347302046D+03	7.981911200D+00	1.003160947D-04	-6.240074170D-08				
1.019540904D-11	-5.698925280D-16		5.830580120D+04	-2.152181937D+01				

Ca(OH)2 Gurvich,1996a pt1 p455 pt2 p358.

2 tpris96 CA	1.000	2.00H	2.00	0.00	0.00	0	74.0926800	-598338.869
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.389257540D+04	-1.791902135D+03	1.621891031D+01	-7.840857170D-03	5.095111610D-06				
-6.955487550D-11	-6.132152640D-13		-6.600405630D+04	-6.070913920D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.721854884D+06	-4.702217670D+03	1.396947691D+01	1.983791405D-04	-1.243050592D-07				
2.033402404D-11	-1.137157819D-15		-4.443761350D+04	-5.287444860D+01				

CaS Gurvich,1996a pt1 p480 pt2 p374.

2 tpris96 CA	1.00S	1.00	0.00	0.00	0.00	0	72.1430000	121475.313
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.320990615D+04	-4.518446080D+02	6.172333750D+00	-3.598852020D-03	4.823731710D-06				
-3.631733540D-09	1.212849867D-12		1.554597691D+04	-7.686936462D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.568353214D+07	5.293855810D+04	-6.322467240D+01	4.027726380D-02	-1.114855081D-05				
1.464389344D-09	-7.376078970D-14		-3.172022670D+05	4.799606012D+02				

Ca2 Gurvich,1996a pt1 p439 pt2 p347.

2 tpris96 CA	2.00	0.00	0.00	0.00	0.00	0	80.1560000	341765.336
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.582228620D+04	1.588188960D+02	1.103952055D+01	-3.333196760D-02	5.345938810D-05				
-4.011573240D-08	1.160486682D-11		3.770350800D+04	-2.397744561D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.405966267D+05	5.775803820D+01	2.347436675D+00	1.199275034D-04	-4.329150310D-08				
7.015302690D-12	-3.705660320D-16		4.081875400D+04	1.895399607D+01				

Cd Hf:Cox,1989. Moore,1971. Gordon,1999.

3 g 7/97 CD	1.00	0.00	0.00	0.00	0.00	0	112.4110000	111800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.081751543D-04	1.816433041D-06	2.499999989D+00	3.129989231D-11	-4.600710160D-14				
3.407048740D-17	-9.989497436D-21		1.270099766D+04	5.931549760D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.699757467D+05	7.866001140D+02	1.628169079D+00	4.594123290D-04	-1.150420443D-07				
1.074836707D-11	8.790199555D-17		7.675148260D+03	1.220006052D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.336284287D+09	9.320949110D+05	-2.490956222D+02	3.302878610D-02	-2.200384347D-06				
7.425712550D-11	-1.026730246D-15		-7.267528990D+06	2.167946107D+03				

Cd+ Moore,1971. Gordon,1999.

3 g 7/97 CD	1.00E	-1.00	0.00	0.00	0.00	0	112.4104514	985754.328
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.098344940D-04	-4.343581620D-06	2.500000019D+00	-4.389036810D-11	5.563969200D-14				
-3.638228260D-17	9.607881995D-21		1.178129439D+05	6.624689450D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.484880812D+04	-4.669153680D+01	2.557883006D+00	-3.624701700D-05	1.213747570D-08				
-2.072802814D-12	1.420665367D-16		1.181070109D+05	6.216414480D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.428364400D+07	4.740395160D+04	-1.165755517D+01	2.220273739D-03	-1.964219980D-07				
9.262295070D-12	-1.560026961D-16		-2.489244513D+05	1.263946278D+02				

CL Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.

3 g 7/97 CL	1.00	0.00	0.00	0.00	0.00	0	35.4530000	121301.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.276215854D+04	-2.168413293D+02	2.745185115D+00	2.451101694D-03	-5.458011990D-06				
4.417986880D-09	-1.288134004D-12		1.501357068D+04	3.102963457D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.697932930D+05	6.081726460D+02	2.128664090D+00	1.307367034D-04	-2.644883596D-08				
2.842504775D-12	-1.252911731D-16		9.934387400D+03	8.844772103D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.139687070D+07	4.499936330D+04	-9.264315350D+00	1.657437964D-03	-1.326219399D-07				
5.533998870D-12	-8.390301878D-17		-3.405333030D+05	1.069111426D+02				

## Appendix D (continued)

CL+ Moore,1971. Moore,1970a. Gordon,1999.

3 g 1/98 CL	1.00E	-1.00	0.00	0.00	0.00	0	35.4524514	1378799.635
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.034697859D+05	-1.293758873D+03	8.186702690D+00	-9.916014600D-03	9.208472370D-06				
-4.507426240D-09	9.182127880D-13		1.714758780D+05	-2.766417931D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.056409480D+04	-4.960165720D+01	3.101653630D+00	-5.868738290D-04	2.252039316D-07				
-3.299703020D-11	1.708780842D-15		1.652982337D+05	2.574942598D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.078099946D+06	-6.858418280D+02	3.092289282D+00	-1.922260015D-05	3.805551560D-10				
-1.571848967D-13	8.442513880D-18		1.683434405D+05	1.334407234D+00				

CL- Hotop,1985. Gordon,1999.

3 g 4/97 CL	1.00E	1.00	0.00	0.00	0.00	0	35.4535486	-233957.972
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-2.888389093D+04	4.200642023D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-2.888389093D+04	4.200642023D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-2.888389093D+04	4.200642023D+00				

CLCN Gurvich,1991 pt1 p230 pt2 p218

2 g 6/95 CL	1.00C	1.00N	1.00	0.00	0.00	0	61.4704000	134200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.274043430D+04	-1.297344947D+03	1.107676527D+01	-1.108430216D-02	1.614009477D-05				
-1.088916772D-08	2.830952246D-12		2.084388986D+04	-3.597370046D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.467573120D+05	-1.957857370D+03	8.807806150D+00	-4.388362780D-04	1.024761895D-07				
-1.110675026D-11	4.986179420D-16		2.581923944D+04	-2.636885363D+01				

CLF Gurvich,1989 pt1 p190 pt2 p97.

2 tpis89 CL	1.00F	1.00	0.00	0.00	0.00	0	54.4514032	-55700.993
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.352210810D+04	-3.688311900D+02	4.272288620D+00	2.549434508D-03	-4.456830890D-06				
3.413854120D-09	-9.838685200D-13		-5.839369690D+03	2.318014199D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.045867173D+06	-9.979328260D+03	1.684162254D+01	-7.465850620D-03	2.336213612D-06				
-3.365865460D-10	1.763082415D-14		5.447120800D+04	-8.707987094D+01				

CLF3 Gurvich,1989 pt1 p193 pt2 p98.

2 tpis89 CL	1.00F	3.00	0.00	0.00	0.00	0	92.4482096	-164600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.285175171D+05	-2.140445721D+03	1.493096474D+01	-6.042471040D-03	3.718968610D-06				
-8.053201100D-10	-7.985600530D-14		-1.138459640D+04	-5.594838353D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.294956235D+05	-1.220741000D+02	1.009124644D+01	-3.649724750D-05	8.058910750D-09				
-9.230849950D-13	4.272569490D-17		-2.282840447D+04	-2.511605479D+01				

CLF5 Gurvich,1989 pt1 p194 pt2 p99.

2 tpis89 CL	1.00F	5.00	0.00	0.00	0.00	0	130.4450160	-238000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.459703939D+05	-4.315348070D+03	2.727005972D+01	-1.670193839D-02	1.421668208D-05				
-6.426479740D-09	1.183099799D-12		-1.071423726D+04	-1.267466837D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.269327450D+05	-2.058057390D+02	1.615465278D+01	-6.212688180D-05	1.376637959D-08				
-1.581335709D-12	7.336422490D-17		-3.361466600D+04	-5.757531175D+01				

CLO Gurvich,1989 pt1 p180 pt2 p90.

2 tpis89 CL	1.000	1.00	0.00	0.00	0.00	0	51.4524000	101621.115
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.687268145D+04	2.573812247D+02	2.175846120D+00	6.432061130D-03	-8.568249500D-06				
5.764971250D-09	-1.545771209D-12		9.829518980D+03	1.386010503D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.093760520D+05	-1.765985112D+03	7.087900630D+00	-1.828450169D-03	7.103818100D-07				
-1.209332942D-10	7.076441040D-15		2.151891784D+04	-1.668645548D+01				

CLO2 Gurvich,1989 pt1 p182 pt2 p91.

2 g 7/93 CL	1.000	2.00	0.00	0.00	0.00	0	67.4518000	105000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.127277696D+04	3.903032030D+02	-3.843018530D-01	2.108677947D-02	-2.793137755D-05				
1.841289286D-08	-4.839779150D-12		9.756933670D+03	2.913262700D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.633793802D+05	-3.161480670D+02	7.009787260D+00	2.837971144D-04	-1.179925338D-07				
2.920383252D-11	-2.024030202D-15		1.184946452D+04	-1.091168827D+01				

## Appendix D (continued)

CL2                      Ref-Elm. Gurvich,1989 pt1 p177 pt2 p88.

2 tpi89 CL	2.00	0.00	0.00	0.00	0.00	0.00	0	70.9060000	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.462815170D+04	-5.547126520D+02	6.207589370D+00	-2.989632078D-03	3.173027290D-06					
-1.793629562D-09	4.260043590D-13			1.534069331D+03	-9.438331107D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.092569420D+06	-1.949627662D+04	2.854535795D+01	-1.449968764D-02	4.463890770D-06					
-6.358525860D-10	3.327360290D-14			1.212117724D+05	-1.690778824D+02				

CL20                      Gurvich,1989 pt1 p184 pt2 p92.

2 tpi89 CL	2.000	1.00	0.00	0.00	0.00	0	86.9054000	79000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.798855400D+04	-1.182537879D+03	9.526514660D+00	-2.596163176D-03	8.696781310D-07				
4.484098270D-10	-3.044511967D-13			1.376729572D+04	-2.484690718D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.271743461D+05	-6.741963220D+01	7.050022450D+00	-1.988084386D-05	4.366209050D-09				
-4.978580680D-13	2.295679186D-17			7.387289300D+03	-8.797477254D+00			

Co                      Hf:Hultgren,1973. Sugar,1985. Gordon,1999.

3 g 7/97 CO	1.00	0.00	0.00	0.00	0.00	0	58.9332000	428441.600
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.598939184D+03	2.461989844D+02	-6.106058370D-01	1.393005772D-02	-2.210012979D-05				
1.623755261D-08	-4.534904351D-12			4.984613760D+04	2.257584199D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.381841305D+06	-3.756036680D+03	6.657130650D+00	-1.269246675D-03	1.464092329D-07				
6.574946570D-12	-1.102384178D-15			7.494442910D+04	-2.258500836D+01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.468015750D+08	4.037704950D+05	-1.142413163D+02	1.663014422D-02	-1.156228007D-06				
3.862515150D-11	-5.002032746D-16			-3.076031798D+06	1.003028648D+03			

Co+                      Sugar,1985. Gordon,1999.

3 g 7/97 CO	1.00E	-1.00	0.00	0.00	0.00	0	58.9326514	1193003.307
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.028494160D+05	-8.744731260D+02	4.279500280D+00	2.225857835D-03	-7.457274570D-06				
7.279221950D-09	-2.347541963D-12			1.474895959D+05	-5.679019220D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.907386174D+06	-8.619705750D+03	1.188134934D+01	-3.510647420D-03	5.748004680D-07				
-2.534065135D-11	-2.976607469D-16			1.977419221D+05	-6.096533440D+01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.701785479D+09	-1.604232092D+06	3.687314770D+02	-4.041150820D-02	2.371848586D-06				
-7.119952160D-11	8.635423717D-16			1.293631390D+07	-3.201662470D+03			

Co-                      Hotop,1985. Gordon,1999.

3 g 9/97 CO	1.00E	1.00	0.00	0.00	0.00	0	58.9337486	358414.372
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.459493760D+04	-1.355041712D+02	1.116330898D+00	9.042761830D-03	-1.454296726D-05				
9.994940630D-09	-2.595633259D-12			4.337037820D+04	1.270494975D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.741394170D+05	1.763109207D+03	1.415561988D+00	3.776869690D-04	-7.534179980D-08				
7.995701540D-12	-3.490440000D-16			3.083493114D+04	1.634360353D+01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.121795840D+05	7.962447120D+02	2.328870839D+00	1.919463732D-05	-1.179708474D-09				
3.764228600D-14	-4.875340940D-19			3.689285080D+04	9.511282720D+00			

Cr                      Hf:Chase,1998 p963 6/79. Sugar,1985. Gordon,1999.

3 g 7/97 CR	1.00	0.00	0.00	0.00	0.00	0	51.9961000	397480.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.335658217D+03	-2.102424026D+01	2.631908173D+00	-4.246263250D-04	7.439194160D-07				
-6.763931630D-10	2.507855625D-13			4.715866640D+04	6.005425450D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.120220789D+07	3.401163690D+04	-3.657062170D+01	2.110296902D-02	-5.518180140D-06				
7.173601710D-10	-3.505127367D-14			-1.688993440D+05	2.864481267D+02			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.900886930D+09	-2.462918543D+06	5.915632640D+02	-6.697121640D-02	3.946957790D-06				
-1.166504597D-10	1.367279456D-15			1.955381984D+07	-5.133510550D+03			

Cr+                      Sugar,1985. Gordon,1999.

3 g 7/97 CR	1.00E	-1.00	0.00	0.00	0.00	0	51.9955514	1056546.728
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.819187467D+02	-2.188843517D+00	2.510676511D+00	-2.706791825D-05	3.768492630D-08				
-2.736784742D-11	8.115389932D-15			1.263380825D+05	6.506276170D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.342330790D+06	-1.064261051D+04	1.557884307D+01	-7.708971480D-03	2.158300274D-06				
-2.368108110D-10	8.952805604D-15			1.932997670D+05	-8.604356670D+01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.853867040D+08	-4.114535830D+05	1.242898882D+02	-1.610102894D-02	1.147677369D-06				
-4.099673600D-11	5.728606039D-16			3.281645810D+06	-1.034723629D+03			

## Appendix D (continued)

Cr- Hotop,1985. Gordon,1999.

3 g10/97 CR	1.00E	1.00	0.00	0.00	0.00	0.00	0.00	51.9966486	327023.428
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						3.858627870D+04	6.566835370D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						3.858627870D+04	6.566835370D+00	
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						3.858627870D+04	6.566835370D+00	

CrN Chase,1998 p967.

2 j12/73 CR	1.00N	1.00	0.00	0.00	0.00	0.00	0.00	66.0028000	505008.800
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.239129220D+03	3.008144202D+02	5.147874920D-01	1.129636791D-02	-1.515183504D-05					
1.010997229D-08	-2.687775750D-12		5.845628120D+04	2.298028696D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.110672490D+06	-3.690478540D+03	8.599056680D+00	-2.125587223D-03	5.282358480D-07					
-4.921139150D-11	1.404331106D-15		8.254804580D+04	-2.799968411D+01					

CrO Gurvich,1982 pt1 p13 pt2 p17.

3 tps82 CR	1.000	1.00	0.00	0.00	0.00	0.00	0.00	67.9955000	186581.318
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.373334110D+03	1.369743818D+02	1.621443428D+00	8.814095960D-03	-1.232845360D-05					
8.497960940D-09	-2.315804197D-12		2.090948871D+04	1.781935787D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.092367332D+06	-3.749758650D+03	9.007870210D+00	-2.545445236D-03	6.928051680D-07					
-6.390831950D-11	1.659741645D-15		4.447098210D+04	-2.942600453D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.600191720D+08	-3.409592350D+05	7.971428300D+01	-7.045904880D-03	3.311256200D-07					
-8.196877430D-12	8.487479810D-17		2.738393714D+06	-6.629641700D+02					

CrO2 Gurvich,1982 pt1 p16 pt2 p19.

2 tps82 CR	1.000	2.00	0.00	0.00	0.00	0.00	0.00	83.9949000	-108043.235
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.548629900D+04	-2.298628537D+02	2.286289393D+00	1.616929338D-02	-2.345198910D-05					
1.631365714D-08	-4.444269620D-12		-1.278912840D+04	1.442954956D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.327109140D+05	1.915584657D+02	7.188247370D+00	-5.694846190D-04	3.546366130D-07					
-5.655123060D-11	2.908946349D-15		-1.743339545D+04	-1.006424720D+01					

CrO3 Gurvich,1982 pt1 p17 pt2 p20.

2 tps82 CR	1.000	3.00	0.00	0.00	0.00	0.00	0.00	99.9943000	-322037.084
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.183020060D+04	-5.059348850D+02	4.432715670D+00	1.995079387D-02	-2.920597649D-05					
2.039330280D-08	-5.580086630D-12		-3.769702400D+04	8.653827280D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.283314010D+05	6.928158180D+02	8.971274600D+00	6.823365640D-04	-2.235048825D-07					
3.366785790D-11	-1.614026492D-15		-4.723880200D+04	-1.945305345D+01					

CrO3- Gurvich,1982 pt1 p18 pt2 p21.

2 tps82 CR	1.000	3.00E	1.00	0.00	0.00	0.00	0.00	99.9948486	-632850.845
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.873455703D+05	-2.300722991D+03	1.343953022D+01	-1.663085846D-03	-1.443973096D-06					
2.045898933D-09	-6.837555300D-13		-6.630111580D+04	-4.930644200D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.499682030D+05	4.522017620D+02	9.980575900D+00	-4.214136730D-04	2.631277945D-07					
-4.594543650D-11	2.659097549D-15		-8.350019730D+04	-2.464810900D+01					

Cs Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.

3 g 7/97 CS	1.00	0.00	0.00	0.00	0.00	0.00	0.00	132.9054500	76500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.466584070D+01	-8.279346040D-01	2.504942210D+00	-1.494620690D-05	2.425976774D-08					
-2.013172322D-11	6.704271991D-15		8.459321390D+03	6.848825772D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.166040900D+06	-1.896175522D+04	2.483229903D+01	-1.251977234D-02	3.309017390D-06					
-3.354012020D-10	9.626500908D-15		1.285111231D+05	-1.522942188D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.566231720D+08	4.321690420D+05	-6.371801020D+01	5.246260580D-03	-2.366560159D-07					
5.848488480D-12	-6.169370441D-17		-3.585268840D+06	6.156618174D+02					

## Appendix D (continued)

Cs+ Moore,1971. Gordon,1999.

3 g 1/98 CS	1.00E	-1.00	0.00	0.00	0.00	0	132.9049014	458401.828
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						5.438737820D+04	6.182757992D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						5.438737820D+04	6.182757992D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.479469300D+08	1.405115456D+05	-2.805027359D+01	3.087928133D-03	-1.273598265D-07				
-3.748818380D-13	1.214944533D-16						-1.072498017D+06	2.756827325D+02

Cs- Hotop,1985. Gordon,1999.

3 g10/97 CS	1.00E	1.00	0.00	0.00	0.00	0	132.9059986	24797.228
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						2.237029001D+03	6.182770382D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						2.237029001D+03	6.182770382D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						2.237029001D+03	6.182770382D+00

CsBO2 Gurvich,1982 pt1 p505 pt2 p526.

2 tpis82 CS	1.00B	1.000	2.00	0.00	0.00	0	175.7152500	-686901.906
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.193609580D+04	-6.664237400D+02	8.134835880D+00	2.902960302D-03	-7.881467920D-07				
-8.327694540D-10	4.441719110D-13						-8.122320070D+04	-1.121622595D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.975579890D+04	-1.656134283D+03	1.116468934D+01	-4.476366990D-04	9.621091810D-08				
-1.081470115D-11	4.938446740D-16						-7.610479670D+04	-3.036616012D+01

CsBr Gurvich,1982 pt1 p490 pt2 p512.

2 tpis82 CS	1.00BR	1.00	0.00	0.00	0.00	0	212.8094500	-206828.875
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.639263647D+03	-6.947477970D+01	4.860058720D+00	-8.587780150D-04	1.375177550D-06				
-9.891766980D-10	2.895433432D-13						-2.589550471D+04	4.465355690D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.528329963D+05	1.259712657D+03	1.704268408D+00	2.776255318D-03	-1.228389838D-06				
2.698111786D-10	-1.983534480D-14						-3.327842030D+04	2.484116659D+01

CsCL Gurvich,1982 pt1 p487 pt2 p509.

2 tpis82 CS	1.00CL	1.00	0.00	0.00	0.00	0	168.3584500	-242228.878
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.538165292D+04	2.972839326D+02	2.667813848D+00	5.583272410D-03	-8.529005090D-06				
6.595191390D-09	-1.989715823D-12						-3.189251450D+04	1.511365709D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.674923480D+06	1.186152941D+04	-1.063287842D+01	9.804117920D-03	-3.277797460D-06				
5.534233390D-10	-3.401231500D-14						-1.048658658D+05	1.114096064D+02

CsF Gurvich,1982 pt1 p483 pt2 p506.

2 tpis82 CS	1.00F	1.00	0.00	0.00	0.00	0	151.9038532	-364214.884
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.843685799D+04	-4.042409390D+02	6.383178860D+00	-4.674323370D-03	6.630134010D-06				
-4.760905530D-09	1.374569797D-12						-4.318489590D+04	-7.226593230D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.850863231D+06	5.625298800D+03	-2.250022212D+00	4.109243540D-03	-1.250243837D-06				
1.941483152D-10	-1.071166179D-14						-8.079827790D+04	5.135559450D+01

CsH Gurvich,1982 pt1 p477 pt2 p501.

2 tpis82 CS	1.00H	1.00	0.00	0.00	0.00	0	133.9133900	115950.106
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.620544411D+04	-7.087016280D+01	2.480847135D+00	7.021985990D-03	-1.007126309D-05				
7.090639030D-09	-1.950395735D-12						1.342777328D+04	9.894247170D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.112146650D+05	3.576472750D+03	-1.258058765D+00	4.314855150D-03	-1.407820502D-06				
2.154598897D-10	-1.254525606D-14						-9.158717270D+03	3.908800030D+01

CsI Gurvich,1982 pt1 p494 pt2 p515.

2 tpis82 CS	1.00I	1.00	0.00	0.00	0.00	0	259.8099200	-152319.873
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.072685650D+03	2.330073667D+01	4.387277690D+00	3.412084290D-04	-2.175588153D-07				
8.906787000D-11	-2.182639837D-15						-1.978766885D+04	8.074657820D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.511259050D+06	-1.341706362D+04	1.980984712D+01	-8.359855550D-03	2.348201245D-06				
-2.874285248D-10	1.208087750D-14						6.573439130D+04	-1.021032592D+02

## Appendix D (continued)

CsLi                      Gurvich,1982 pt1 p505 pt2 p527.  
 2 tpris82 CS 1.00LI 1.00 0.00 0.00 0.00 0 139.8464500 162146.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10341.124  
 1.368709568D+03-7.451297060D+01 4.845620930D+00-5.573667210D-04 4.953326760D-07  
 4.369068910D-10-4.608145770D-13 1.850577392D+04 2.112012017D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10341.124  
 7.481630230D+06-2.885297839D+04 4.631104990D+01-2.784288108D-02 8.787413490D-06  
 -1.264901197D-09 6.720186280D-14 1.945137819D+05-2.857846194D+02

CsNO2                      Gurvich,1982 pt1 p499 pt2 p520.  
 2 tpris82 CS 1.00N 1.000 2.00 0.00 0.00 0 178.9109500 -210339.828  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15980.172  
 -7.106010440D+04 1.272448257D+03-2.447362349D+00 3.064441948D-02-3.699225940D-05  
 2.259121812D-08-5.580635910D-12 -3.313370920D+04 4.954693336D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15980.172  
 -1.633503154D+05-8.468879580D+02 1.062853461D+01-2.508799215D-04 5.541255770D-08  
 -6.355591950D-12 2.946880031D-16 -2.403040739D+04-2.443488888D+01

CsNO3                      Gurvich,1982 pt1 p501 pt2 p522.  
 2 tpris82 CS 1.00N 1.000 3.00 0.00 0.00 0 194.9103500 -318486.390  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16563.610  
 -2.677219779D+04 9.011692690D+02-3.265340820D+00 4.298377700D-02-5.386751380D-05  
 3.384527520D-08-8.565223660D-12 -4.405304140D+04 5.118862689D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16563.610  
 -3.147517676D+05-1.367011655D+03 1.401012848D+01-4.018647130D-04 8.853614700D-08  
 -1.013466457D-11 4.691758730D-16 -3.549026670D+04-4.500692791D+01

CsNa                      Gurvich,1982 pt1 p506 pt2 p528.  
 2 tpris82 CS 1.00NA 1.00 0.00 0.00 0.00 0 155.8952200 125907.329  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10702.129  
 2.521738609D+04-4.295362490D+02 7.223094740D+00-8.460463000D-03 1.443905157D-05  
 -1.143624855D-08 3.183721930D-12 1.579099265D+04-8.838790300D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10702.129  
 3.879556790D+06-1.780167288D+04 3.491355800D+01-2.320080793D-02 7.861975840D-06  
 -1.171011257D-09 6.323927370D-14 1.195776556D+05-2.001754433D+02

CsO                      Gurvich,1982 pt1 p471 pt2 p493.  
 2 tpris82 CS 1.00O 1.00 0.00 0.00 0.00 0 148.9048500 37587.318  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9835.118  
 8.683958810D+03 4.250278170D+02-3.484055300D+00 3.801969830D-02-6.651927560D-05  
 5.173472190D-08-1.512567066D-11 1.969690015D+03 4.240796140D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9835.118  
 8.375544350D+05-2.418205772D+03 8.908065350D+00-3.378180040D-03 1.312755917D-06  
 -2.150508925D-10 1.219138980D-14 1.809493447D+04-2.460858580D+01

CsOH                      Gurvich,1997.  
 2 g 9/97 CS 1.00O 1.00H 1.00 0.00 0.00 0 149.9127900 -256000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11834.689  
 9.386960790D+03-5.009354260D+02 8.301351980D+00-3.235596840D-03 2.612406777D-06  
 -4.950613410D-10-1.038364927D-13 -3.025722427D+04-1.742194837D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11834.689  
 8.967171130D+05-2.323978587D+03 7.959644870D+00 1.101149275D-04-6.466013970D-08  
 1.045968201D-11-5.822514170D-16 -1.736258234D+04-1.864239624D+01

CsRb                      Gurvich,1982 pt1 p508 pt2 p530.  
 2 tpris82 CS 1.00RB 1.00 0.00 0.00 0.00 0 218.3732500 111477.332  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10972.132  
 -4.910922680D+03-9.209015550D+00 5.193377890D+00-4.390246990D-03 1.254790436D-05  
 -1.414878514D-08 5.101441310D-12 1.200498171D+04 5.361542930D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10972.132  
 -1.328693378D+07 3.414579470D+04-2.373696406D+01 7.070465400D-03 3.863450970D-07  
 -3.158132986D-10 2.667747207D-14 -2.124008997D+05 2.239970251D+02

Cs2                      Gurvich,1982 pt1 p467 pt2 p492.  
 2 tpris82 CS 2.00 0.00 0.00 0.00 0.00 0 265.8109000 109404.333  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11029.133  
 -4.674158730D+04 5.952019510D+02 1.895333975D+00 4.082065810D-03 2.531487119D-06  
 -9.085139030D-09 4.290179930D-12 8.857282570D+03 2.391592727D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11029.133  
 -2.592739590D+07 7.539818910D+04-7.484086800D+01 3.692866790D-02-8.082497240D-06  
 8.171850730D-10-3.089285900D-14 -4.715045720D+05 5.860933750D+02

## Appendix D (continued)

Cs2Br2                      Gurvich,1982 pt1 p491 pt2 p513.  
 2 tpris82 CS    2.00BR    2.00    0.00    0.00    0.00 0    425.6189000    -565828.869  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22113.130  
 -6.321285180D+03-1.213153529D+01 1.004967112D+01-1.102100044D-04 1.365293456D-07  
 -8.856957070D-11 2.339447704D-14                      -7.099771710D+04-7.539424790D+00  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22113.130  
 -7.545846650D+03-2.087093009D-01 1.000018042D+01-8.034260730D-08 1.923604258D-11  
 -2.344698140D-15 1.139365834D-19                      -7.105883540D+04-7.251793040D+00

Cs2CO3                      Gurvich,1982 pt1 p503 pt2 p524.  
 2 tpris82 CS    2.00C    1.000    3.00    0.00    0.00 0    325.8198000    -806447.939  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    21179.061  
 -4.673130000D+04 9.436549060D+02-2.374670436D-01 4.168484610D-02-5.094372210D-05  
   3.132078394D-08-7.780421670D-12                      -1.039162411D+05 4.055853980D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    21179.061  
 -3.037149985D+05-1.517078400D+03 1.711941656D+01-4.449700120D-04 9.798325240D-08  
 -1.121256063D-11 5.189734780D-16                      -9.420414770D+04-5.682006260D+01

Cs2CL2                      Gurvich,1982 pt1 p487 pt2 p510.  
 2 tpris82 CS    2.00CL    2.00    0.00    0.00    0.00 0    336.7169000    -644658.398  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    20944.712  
 -1.077956357D+04-5.346106950D+01 1.021710683D+01-4.789687030D-04 5.908946530D-07  
 -3.821416520D-10 1.006995985D-13                      -8.029515170D+04-1.207856486D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    20944.712  
 -1.625143966D+04-9.006137350D-01 1.000077173D+01-3.416194080D-07 8.144968080D-11  
 -9.897475280D-15 4.798330810D-19                      -8.056513220D+04-1.081977337D+01

Cs2F2                      Gurvich,1982 pt1 p484 pt2 p507.  
 2 tpris82 CS    2.00F    2.00    0.00    0.00    0.00 0    303.8077064    -891858.506  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    19388.600  
 -9.942677480D+03-2.536723355D+02 1.100684073D+01-2.185640152D-03 2.664791874D-06  
 -1.708229209D-09 4.471151980D-13                      -1.090582601D+05-2.000699602D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    19388.600  
 -3.677946420D+04-4.355753480D+00 1.000366687D+01-1.603814186D-06 3.791469740D-10  
 -4.578687430D-14 2.209385787D-18                      -1.103456448D+05-1.415086452D+01

Cs2I2                      Gurvich,1982 pt1 p495 pt2 p516.  
 2 tpris82 CS    2.00I    2.00    0.00    0.00    0.00 0    519.6198400    -454033.097  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22584.903  
 -4.449286970D+03-5.321793660D+00 1.002183919D+01-4.853374850D-05 6.019338400D-08  
 -3.908226390D-11 1.032981014D-14                      -5.757823380D+04-5.271267090D+00  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22584.903  
 -4.983376010D+03-9.461179880D-02 1.000008229D+01-3.680962040D-08 8.844660910D-12  
 -1.081178562D-15 5.266141980D-20                      -5.760501040D+04-5.144864890D+00

Cs2O                      Gurvich,1982 pt1 p473 pt2 p496.  
 2 tpris82 CS    2.00O    1.00    0.00    0.00    0.00 0    281.8103000    -142855.345  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14089.855  
   1.910533804D+04-4.962181530D+02 8.759606300D+00-3.511622790D-03 4.016479830D-06  
 -2.450899853D-09 6.172404890D-13                      -1.677664956D+04-1.159258822D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14089.855  
 -4.119147410D+04-1.079255391D+01 7.008500470D+00-3.542955780D-06 8.081699120D-10  
 -9.499419930D-14 4.489122540D-18                      -1.934377850D+04-1.203970450D+00

Cs2O+                      Gurvich,1982 pt1 p474 pt2 p497.  
 2 tpris82 CS    2.00O    1.00E -1.00    0.00    0.00 0    281.8097514    283699.926  
   298.150    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14447.726  
   6.837056090D+02-2.435575007D+02 7.783037470D+00-1.414552725D-03 1.470799739D-06  
 -8.218821330D-10 1.911749489D-13                      3.324194870D+04-4.750423560D+00  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14447.726  
 -3.153085844D+04-5.771559030D+00 7.004482630D+00-1.848241331D-06 4.180882300D-10  
 -4.882376270D-14 2.295419936D-18                      3.196227310D+04-5.434350690D-02

Cs2O2                      Gurvich,1982 pt1 p476 pt2 p499.  
 2 tpris82 CS    2.00O    2.00    0.00    0.00    0.00 0    297.8097000    -247069.104  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17426.496  
   2.274505180D+04-5.667912570D+02 1.001728332D+01 2.547081016D-03-4.909216690D-06  
   3.848788910D-09-1.124566008D-12                      -2.947334360D+04-1.841275291D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    17426.496  
 -1.190032094D+05-9.261075260D+01 1.006915777D+01-2.766227147D-05 6.110752960D-09  
 -7.003595480D-13 3.243742520D-17                      -3.255610740D+04-1.724868948D+01



## Appendix D (continued)

Cs2O2H2 Gurvich, 1997.

2 g 9/97 CS	2.000	2.00H	2.00	0.00	0.00	0	299.8255800	-653000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-1.085981041D+04	-6.883068420D+02	1.643543354D+01	-4.039220580D-03	2.331117156D-06				
8.439651630D-10	-6.859309730D-13		-7.939476230D+04	-4.906196810D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
1.802857941D+06	-4.656354750D+03	1.693566597D+01	2.117402535D-04	-1.272249096D-07				
2.066555839D-11	-1.152390667D-15		-5.190813690D+04	-5.849719160D+01				

Cs2SO4 Gurvich, 1982 pt1 p497 pt2 p518.

2 g10/99 CS	2.00S	1.000	4.00	0.00	0.00	0	361.8735000	-1117651.834
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
6.153637870D+04	-6.381374330D+02	6.894772090D+00	3.960182910D-02	-5.529862010D-05				
3.736332520D-08	-9.973241830D-12		-1.339760310D+05	-1.284432588D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-5.223397520D+05	-9.444155250D+02	1.970476453D+01	-2.821225990D-04	6.240792280D-08				
-7.163464070D-12	3.322667190D-16		-1.364179983D+05	-6.820406795D+01				

Cu Hf: Cox, 1989. Sugar, 1990. Gordon, 1999.

3 g12/97 CU	1.00	0.00	0.00	0.00	0.00	0	63.5460000	337400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
7.71313150D+01	-1.169236206D+00	2.506987803D+00	-2.116434879D-05	3.441714710D-08				
-2.862608999D-11	9.559250991D-15		3.983981210D+04	5.730813220D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
2.308090411D+06	-8.503261000D+03	1.467859102D+01	-8.467136520D-03	2.887821016D-06				
-4.270659180D-10	2.304265084D-14		9.207535620D+04	-7.854701560D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-6.490595890D+08	4.240323360D+05	-1.028965806D+02	1.297259934D-02	-7.766697680D-07				
2.220446727D-11	-2.441532031D-16		-3.305304580D+06	9.198622920D+02				

Cu+ Sugar, 1990. Gordon, 1999.

3 g 3/98 CU	1.00E	-1.00	0.00	0.00	0.00	0	63.5454514	1089079.728
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-2.452340093D-03	2.606893531D-05	2.499999890D+00	2.351922485D-10	-2.669362382D-13				
1.510315123D-16	3.278224814D-20		1.302400621D+05	5.075940770D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-2.181443016D+06	7.217858190D+03	-6.941154750D+00	6.208248920D-03	-2.139340497D-06				
3.566431440D-10	-2.081198501D-14		8.516456660D+04	7.116800670D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
2.994686480D+09	-1.831416099D+06	4.294926960D+02	-4.801927720D-02	2.836504248D-06				
-8.452189040D-11	1.013018211D-15		1.468809255D+07	-3.729918010D+03				

Cu- Hotop, 1985. Gordon, 1999.

3 g10/97 CU	1.00E	1.00	0.00	0.00	0.00	0	63.5465486	212718.628
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		2.483864954D+04	5.075966030D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		2.483864954D+04	5.075966030D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		2.483864954D+04	5.075966030D+00				

CuCL Chase, 1998 p748.

2 j 3/66 CU	1.00CL	1.00	0.00	0.00	0.00	0	98.9990000	91090.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
1.469847736D+04	-3.393167250D+02	5.723459590D+00	-2.417296132D-03	2.858019864D-06				
-1.757900548D-09	4.455047290D-13		1.131714015D+04	-4.527352594D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-2.577122410D+04	-7.106346060D+00	4.505623180D+00	5.394548270D-05	5.386417960D-10				
-6.348482770D-14	3.006622062D-18		9.566192870D+03	2.680067564D+00				

CuF Chase, 1998 p1013.

2 j12/77 CU	1.00F	1.00	0.00	0.00	0.00	0	82.5444032	-12550.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
3.761385410D+04	-5.468104900D+02	5.832351720D+00	-1.695312068D-03	1.218150880D-06				
-3.713285280D-10	2.002276589D-14		5.865140720D+01	-7.156930090D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
5.094154830D+05	-1.415009870D+03	5.632349380D+00	-1.629128410D-04	-1.156611499D-07				
5.066034080D-11	-4.153205110D-15		6.305506600D+03	-7.407773610D+00				

## Appendix D (continued)

CuF2 Chase,1998 p1017.

2 j12/77 CU	1.00F	2.00	0.00	0.00	0.00	0.00	0.00	101.5428064	-266940.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.573311280D+04	-8.962430840D+02	7.917560940D+00	1.345667904D-03	-4.162400010D-06					
3.716181090D-09	-1.155537597D-12		-2.916887325D+04	-1.587076153D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.650355082D+06	3.775362120D+03	3.889116550D+00	6.821912640D-04	1.875979026D-07					
-5.677368110D-11	3.823248730D-15		-5.953371700D+04	1.522659664D+01					

CuO Chase,1998 p1020.

2 j12/77 CU	1.00O	1.00	0.00	0.00	0.00	0.00	0.00	79.5454000	306270.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.689762240D+03	-1.184808464D+02	4.566155240D+00	4.309058020D-04	-8.309886400D-07					
6.946638020D-10	-2.108693366D-13		3.615190680D+04	1.733847344D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.582280170D+05	-9.139366410D+02	5.136898670D+00	6.240577240D-05	-1.558613495D-07					
5.236803120D-11	-4.026745620D-15		4.150792860D+04	-2.634070960D+00					

Cu2 Chase,1998 p1022.

2 j 9/66 CU	2.00	0.00	0.00	0.00	0.00	0.00	0.00	127.0920000	485340.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.529183480D+02	-9.720044930D+01	4.882233700D+00	-7.371369400D-04	1.000575401D-06					
-6.391989440D-10	1.668655797D-13		5.749307020D+04	1.105391325D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.699399500D+04	3.209103870D+02	3.973802880D+00	5.080809670D-04	-1.707470385D-07					
3.219108190D-11	-1.958830868D-15		5.506090190D+04	6.914502170D+00					

Cu3CL3 Chase,1998 p874.

2 j 3/66 CU	3.00CL	3.00	0.00	0.00	0.00	0.00	0.00	296.9970000	-258570.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.487885320D+03	-8.736644440D+02	1.936189091D+01	-7.137447860D-03	8.560454870D-06					
-5.419978740D-09	1.405175350D-12		-3.162689960D+04	-5.976797945D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.188559680D+04	-1.571936430D+01	1.601294170D+01	-5.572992370D-06	1.302748507D-09					
-1.560175322D-13	7.480827570D-18		-3.608760740D+04	-4.013211395D+01					

D D0 (D2): Herzberg,1970. Moore,1972. Gordon,1999.

3 g 6/97 D	1.00	0.00	0.00	0.00	0.00	0.00	0.00	2.0141020	221720.228
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		2.592128700D+04	5.917143380D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.050019210D+01	-1.810766064D-01	2.500210817D+00	-1.220711706D-07	3.715172170D-11					
-5.660680210D-15	3.393920393D-19		2.592243752D+04	5.902125370D-01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.169259778D+08	-1.309309862D+05	3.392595050D+01	-3.805973810D-03	2.427699393D-07					
-7.677967800D-12	9.624191177D-17		1.065922040D+06	-2.726201602D+02					

D+ Moore,1972. Gordon,1999.

3 g 9/96 D	1.00E	-1.00	0.00	0.00	0.00	0.00	0.00	2.0135534	1540324.328
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		1.845120037D+05	-1.018414521D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		1.845120037D+05	-1.018414521D-01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		1.845120037D+05	-1.018414521D-01					

D- Hotop,1985. Gordon,1999.

3 g 8/96 D	1.00E	1.00	0.00	0.00	0.00	0.00	0.00	2.0146506	142752.728
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		1.642373393D+04	-1.010243437D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		1.642373393D+04	-1.010243437D-01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	
0.000000000D+00	0.000000000D+00		1.642373393D+04	-1.010243437D-01					

## Appendix D (continued)

DBr Gurvich,1989 pt1 p206 pt2 p107.

2 tpis89 D	1.00BR	1.00	0.00	0.00	0.00	0.00	0	81.9181020	-37036.496
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.918282458D+04	2.020175399D+02	3.044629038D+00	-1.488157450D-03	6.870897800D-06					
-6.591160280D-09	2.093769216D-12			-6.560074400D+03	8.008690040D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.654000440D+05	-2.594092228D+03	6.885879400D+00	-1.103284901D-03	2.894201105D-07					
-3.152037514D-11	1.011011776D-15			1.037813140D+04	-1.973703653D+01				

DCL Gurvich,1989 pt1 p188 pt2 p95.

2 tpis89 D	1.00CL	1.00	0.00	0.00	0.00	0	37.4671020	-93547.003	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.046421033D+04	-2.313813446D+02	5.420693260D+00	-7.508012650D-03	1.398672495D-05					
-1.066249569D-08	3.011167635D-12			-1.128403374D+04	-6.711842349D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.117284900D+05	-1.764535217D+03	5.668877100D+00	-3.475964170D-04	5.882688030D-08					
3.760253130D-13	-5.164600560D-16			-1.541258092D+03	-1.275659404D+01				

DF Gurvich,1989 pt1 p172 pt2 p80.

3 tpis89 D	1.00F	1.00	0.00	0.00	0.00	0	21.0125052	-276227.596	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.721370750D+04	-7.311733800D+02	7.220870870D+00	-9.423969350D-03	1.208025139D-05					
-6.941812690D-09	1.538525476D-12			-3.069230024D+04	-1.932760992D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.001172800D+05	-2.438386832D+03	5.620664450D+00	-2.020416838D-04	1.714418979D-08					
2.697462563D-12	-2.888297410D-16			-1.857447029D+04	-1.473004444D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.924190104D+08	-9.333761700D+04	1.929651319D+01	-6.429319300D-04	-1.978551386D-08					
1.730048706D-12	-3.030499069D-17			7.325924600D+05	-1.428958225D+02				

DOCL D0 estimated from HOCL. Jacox,1998 p155.

2 g 1/01 D	1.000	1.00CL	1.00	0.00	0.00	0	53.4665020	-79538.686	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.852834290D+04	-7.673444550D+02	5.933970140D+00	2.868820667D-03	-5.207166370D-06					
4.927572740D-09	-1.709526276D-12			-6.824035050D+03	-7.757833983D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.043066330D+05	-2.646500381D+03	8.612474210D+00	-5.532268240D-04	1.086845232D-07					
-1.137381290D-11	4.904295520D-16			4.845795180D+03	-2.588861801D+01				

DO2 Gurvich,1989 pt1 p138 pt2 p49.

2 tpis89 D	1.000	2.00	0.00	0.00	0.00	0	34.0129020	6487.344	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.111479735D+04	6.023371750D+02	-1.294877674D+00	1.812947970D-02	-2.161807666D-05					
1.391729127D-08	3.697740280D-12			-2.976943856D+03	3.272834480D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.267224927D+06	2.799947016D+03	2.325174609D+00	2.726325070D-03	-6.314507320D-07					
6.729289200D-11	-2.765192818D-15			-1.959411733D+04	1.789922833D+01				

DO2- Gurvich,1989 pt1 p139 pt2 p50.

2 tpis89 D	1.000	2.00E	1.00	0.00	0.00	0	34.0134506	-104795.510	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.048705051D+05	-8.906236770D+02	5.666553560D+00	1.904603784D-03	-1.215263210D-06					
6.577513330D-10	-2.147376147D-13			-8.942377250D+03	-7.797219200D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.527661920D+05	-2.796895783D+03	8.772206670D+00	-6.291116630D-04	1.272331622D-07					
-1.364440687D-11	6.005199440D-16			2.512066767D+03	-2.890020381D+01				

D2 Ref-Species. Gurvich,1989 pt1 p134 pt2 p45.

3 tpis89 D	2.00	0.00	0.00	0.00	0.00	0	4.0282040	0.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.125790482D+04	-2.996945907D+02	5.130314980D+00	-4.172970890D-03	5.014345720D-06					
-2.126389969D-09	2.386536969D-13			3.944985900D+02	-1.164191209D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.215168560D+05	-2.365623159D+03	5.342974510D+00	6.928145990D-05	-8.523671020D-08					
2.456447415D-11	-1.960597698D-15			1.434214587D+04	-1.712600356D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.899848740D+08	-3.112892916D+05	7.945961340D+01	-8.425828740D-03	4.789458020D-07					
-1.390917969D-11	1.637606941D-16			2.460108052D+06	-6.637009520D+02				

D2+ Chase,1998 p1041.

2 j 9/77 D	2.00E	-1.00	0.00	0.00	0.00	0	4.0276554	1498568.325	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.640959090D+04	1.243052385D+03	-2.557714366D+00	1.343064234D-02	-1.285600289D-05					
6.463421670D-09	-1.337616868D-12			1.730966171D+05	3.356314920D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.255951350D+05	-4.505219940D+03	1.103203365D+01	-4.706089030D-03	1.838068460D-06					
-3.135924623D-10	1.857684975D-14			2.058298890D+05	-5.283912240D+01				

## Appendix D (continued)

D2- Chase,1998 p1042.

2 j 9/77 D	2.00E	1.00	0.00	0.00	0.00	0.00	0.00	4.0287526	235160.621
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.365332060D+03	3.112987057D+02	5.481950030D-01	9.956988110D-03	-1.167000612D-05					
6.975656410D-09	-1.682718179D-12		2.597897625D+04	1.442223161D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.798805190D+04	-3.122959355D+02	4.730388280D+00	5.695900800D-05	2.018975430D-08					
-2.311492448D-12	1.070266527D-16		2.851200896D+04	-9.157527920D+00					

D2O Gurvich,1989 pt1 p142 pt2 p51.

2 g 6/99 D	2.000	1.00	0.00	0.00	0.00	0.00	0.00	20.0276040	-249210.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.958278470D+03	-1.280889437D+01	3.595878870D+00	1.502093683D-03	3.594675050D-07					
5.340417200D-10	-5.181941270D-13		-3.101944566D+04	2.895556576D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.544193253D+06	-5.474238900D+03	1.017542424D+01	-9.619415540D-04	2.036545675D-07					
-2.050566442D-11	1.510770690D-16		2.983248980D+03	-4.465011570D+01					

D2O2 Gurvich,1989 pt1 p142 pt2 p52.

2 g 6/99 D	2.000	2.00	0.00	0.00	0.00	0.00	0.00	36.0270040	-144300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.957711324D+04	-6.893037570D+01	2.043905473D+00	1.570281822D-02	-1.935478714D-05					
1.384941336D-08	-4.104184900D-12		-1.802502679D+04	1.347156482D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.147867936D+06	-5.225760930D+03	1.311088701D+01	-1.179811896D-03	2.729336904D-07					
-2.961433535D-11	1.310306129D-15		1.219580532D+04	-5.690538200D+01					

D2S Miller,1967. H2S data.

2 g 6/01 D	2.00S	1.00	0.00	0.00	0.00	0.00	0.00	36.0932040	-24006.550
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.988386480D+03	-6.620792560D+01	4.393354450D+00	-2.325113084D-03	1.189503465D-05					
-1.146524521D-08	3.626190450D-12		-3.787385550D+03	9.238754375D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.235814630D+05	-2.823776231D+03	8.962821840D+00	-6.469231230D-04	1.634615644D-07					
-1.797991376D-11	8.160939570D-16		1.204603509D+04	-3.191047376D+01					

F Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.

3 g 5/97 F	1.00	0.00	0.00	0.00	0.00	0.00	0.00	18.9984032	79380.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.137409088D+03	-1.453392797D+02	4.077403610D+00	-4.303360140D-03	5.728897740D-06					
-3.819312900D-09	1.018322509D-12		9.311110120D+03	-3.558982650D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.473506226D+04	8.149927360D+01	2.444371819D+00	2.120210026D-05	-4.546918620D-09					
5.109528730D-13	-2.333894647D-17		8.388374650D+03	5.478710640D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.926724756D+07	1.775674924D+04	-1.814463258D+00	5.351200280D-04	-3.513620800D-08					
1.101519690D-12	-1.061293837D-17		-1.319642721D+05	4.248814560D+01					

F+ Moore,1971. Moore,1970a. Gordon,1999.

3 g 3/97 F	1.00E	-1.00	0.00	0.00	0.00	0.00	0.00	18.9978546	1766816.332
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.871680190D+04	3.218815660D+02	2.200920452D+00	-2.455492688D-04	7.858355060D-07					
-6.435987920D-10	1.839793564D-13		2.098830937D+05	7.816999240D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.649635664D+04	1.337351478D+02	2.332522942D+00	1.215277877D-04	-4.801037700D-08					
9.027225150D-12	-5.470664940D-16		2.110745327D+05	6.625817090D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.599619330D+06	-1.391106563D+03	1.714871534D+00	2.428311844D-04	-1.894860146D-08					
6.420828070D-13	-8.257979730D-18		2.269126001D+05	1.102848944D+01					

F- Hotop,1985. Gordon,1999.

3 g 1/98 F	1.00E	1.00	0.00	0.00	0.00	0.00	0.00	18.9989518	-255092.072
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-3.142572443D+04	3.264882710D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-3.142572443D+04	3.264882710D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-3.142572443D+04	3.264882710D+00					

## Appendix D (continued)

FCN Gurvich,1991 pt1 p229 pt2 p217.

2 g 5/99 F	1.00C	1.00N	1.00	0.00	0.00	0	45.0158032	34327.854
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.984454120D+04	-6.988655360D+02	7.058839660D+00	-1.404863382D-03	3.964652510D-06				
-3.045609294D-09	7.923045900D-13		6.172627570D+03	-1.505643174D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.981873550D+05	-2.302971079D+03	9.027081390D+00	-5.228710260D-04	1.191059272D-07				
-1.280287231D-11	5.733807190D-16		1.588449451D+04	-2.984971982D+01				

FCO Hf:Gurvich,1991 pt1 p87. Jacox,1998 p193.

2 g12/99 F	1.00C	1.00O	1.00	0.00	0.00	0	47.0085032	-179418.150
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.132662744D+04	-5.397918500D+01	2.966927601D+00	7.559959350D-03	-6.211773580D-06				
2.403781550D-09	-3.369507750D-13		-2.240369579D+04	1.092652142D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.085851580D+04	-1.022397533D+03	7.527322560D+00	-1.057942328D-04	-1.365311093D-09				
2.484612871D-12	-9.997916800D-17		-1.805098416D+04	-1.630331278D+01				

FO Chase,1996b p582.

2 j 9/95 F	1.00O	1.00	0.00	0.00	0.00	0	34.9978032	109012.100
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.912182440D+04	7.967036940D+02	-1.634777767D+00	1.601810071D-02	-2.095210771D-05				
1.382740666D-08	-3.664524950D-12		8.375525230D+03	3.383325720D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.597940503D+06	4.377376380D+03	-4.897507640D-01	2.682336321D-03	-6.900804850D-07				
7.246479680D-11	-2.726912632D-15		-1.644248211D+04	3.559923610D+01				

FO2,FOO Chase,1996b p582.

2 j 9/95 F	1.00O	2.00	0.00	0.00	0.00	0	50.9972032	25400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.821564000D+03	-2.347363967D+02	5.437338760D+00	2.165855252D-03	3.671472190D-07				
-2.071530827D-09	9.431066850D-13		2.694856027D+03	-1.168202057D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.213166895D+06	2.493397189D+03	4.465065740D+00	9.416104040D-04	-6.426472260D-08				
-1.085643277D-11	1.216995394D-15		-1.596800286D+04	8.655193180D+00				

FO2,OFO Chase,1996b p583.

2 j 9/95 F	1.00O	2.00	0.00	0.00	0.00	0	50.9972032	378600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.734106400D+04	1.663800209D+03	-9.612815160D+00	4.989156870D-02	-6.946217130D-05				
4.707787800D-08	-1.258890729D-11		3.697092730D+04	7.795943040D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.211867340D+05	9.369474590D+02	6.401558750D+00	2.136110846D-04	-4.337977650D-08				
4.667312240D-12	-2.059767432D-16		3.638357270D+04	-6.150264330D+00				

F2 Ref-Elm. Gurvich,1989. pt1 p157 pt2 p73.

2 tpis89 F	2.00	0.00	0.00	0.00	0.00	0	37.9968064	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
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
-2.941167790D+06	9.456597700D+03	-7.738616150D+00	7.644712990D-03	-2.241007605D-06				
2.915845236D-10	-1.425033974D-14		-6.071005610D+04	8.423835080D+01				

F2O Gurvich,1989 pt1 p161 pt2 p76.

2 g 4/99 F	2.00O	1.00	0.00	0.00	0.00	0	53.9962064	24500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.082919995D+04	-2.299506259D+02	2.603805825D+00	1.586111264D-02	-2.345633734D-05				
1.679619314D-08	-4.703560330D-12		3.055185332D+03	1.050933022D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.885374518D+05	-2.100729689D+02	7.151239160D+00	1.327687906D-04	1.804705706D-08				
-1.416973671D-12	6.489389390D-17		1.449129965D+03	-1.257858336D+01				

F2O2 FOOF. Chase,1996b p585.

2 j 9/95 F	2.00O	2.00	0.00	0.00	0.00	0	69.9956064	19200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.612270460D+04	-9.985952230D+02	8.980649390D+00	6.421900870D-03	-9.888516020D-06				
6.858061010D-09	-1.842137493D-12		5.298712590D+03	-2.239292195D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.190563532D+05	-3.910920810D+02	1.029107144D+01	-1.163345202D-04	2.570922521D-08				
-2.949199983D-12	1.367386916D-16		8.278020940D+02	-2.756752555D+01				

## Appendix D (continued)

FS2F                      Difluorodisulfane. Chase,1998 p1146.

2 j 6/76 F	2.00S	2.00	0.00	0.00	0.00	0.00	0	102.1268064	-336435.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.144462280D+05	-1.853247564D+03	1.394098518D+01	-4.043689370D-03	1.370970316D-06					
6.711903100D-10	-4.624954960D-13							-3.351068330D+04	-4.849215357D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.077097921D+05	-1.094539831D+02	1.008136946D+01	-3.239537910D-05	7.125225270D-09					
-8.134787410D-13	3.755022410D-17							-4.349446060D+04	-2.346916058D+01

Fe                      Hf:Hultgren,1973. Sugar,1985. Gordon,1999.

3 g 5/97 FE	1.00	0.00	0.00	0.00	0.00	0	55.8450000	415471.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.790822660D+04	-1.197218407D+03	9.843393310D+00	-1.652324828D-02	1.917939959D-05					
-1.149825371D-08	2.832773807D-12							5.466995940D+04	-3.383946260D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.954923682D+06	6.737161100D+03	-5.486410970D+00	4.378803450D-03	-1.116286672D-06					
1.544348856D-10	8.023578182D-15							7.137370060D+03	6.504979860D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.216352511D+09	-5.828563930D+05	9.789634510D+01	-5.370704430D-03	3.192037920D-08					
6.267671430D-12	-1.480574914D-16							4.847648290D+06	-8.697289770D+02

Fe+                      Sugar,1985. Gordon,1999.

3 g 3/98 FE	1.00E	-1.00	0.00	0.00	0.00	0	55.8444514	1184217.849	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.691231620D+04	1.847134390D+02	4.196972120D+00	-5.978275970D-03	1.054267912D-05					
-8.059804320D-09	2.256925874D-12							1.401206571D+05	-3.602542580D-01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.176450090D+05	1.925359408D+03	1.717387154D+00	3.385338980D-04	-9.813533120D-08					
2.228179208D-11	-1.483964439D-15							1.286352466D+05	1.500256262D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.065217491D+08	-2.883923997D+04	-2.821752459D+00	2.712846797D-03	-3.107069182D-07					
1.543726493D-11	-2.725133516D-16							4.142981690D+05	4.053497330D+01

Fe-                      Hotop,1985. Gordon,1999.

3 g 9/97 FE	1.00E	1.00	0.00	0.00	0.00	0	55.8455486	393338.036	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.341276767D+05	-1.775438064D+03	1.084366935D+01	-1.499440282D-02	1.412129744D-05					
-6.942189050D-09	1.410953082D-12							5.519472530D+04	-4.140886490D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.237808631D+05	8.249279070D+02	1.912936452D+00	2.280194065D-04	-4.942014160D-08					
5.591493490D-12	-2.566386941D-16							4.156251610D+04	1.265367627D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.116600852D+06	7.642402360D+02	2.332880311D+00	1.892649914D-05	-1.170322571D-09					
3.749758920D-14	-4.871021520D-19							4.111417150D+04	9.680921840D+00

Fe(CO)5                      Chase,1998 p698.

2 j 3/78 FE	1.00C	5.000	5.00	0.00	0.00	0	195.8955000	-727850.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.797805710D+05	-7.285928160D+03	5.400236180D+01	-6.935400750D-02	1.026705717D-04					
-7.207373130D-08	1.958981996D-11							-5.854580480D+04	-2.604377836D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.116600852D+06	8.067074730D+03	3.652942410D+01	-2.047190300D-03	4.441967750D-07					
-4.932507130D-11	2.235704865D-15							-4.860661250D+04	-1.754566113D+02

FeCL                      Chase,1998 p761.

2 j 6/65 FE	1.00CL	1.00	0.00	0.00	0.00	0	91.2980000	251040.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.117340353D+04	-5.402144290D+01	3.486057920D+00	6.879837140D-03	-1.273679557D-05					
1.025321859D-08	-3.051544011D-12							2.928681990D+04	9.428962979D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.288700220D+05	-1.282897413D+03	5.798441690D+00	-2.896589776D-04	3.343903810D-08					
-1.469606582D-13	-1.213444602D-16							3.726196730D+04	-4.075134191D+00

FeCL2                      Chase,1998 p822.

2 j12/70 FE	1.00CL	2.00	0.00	0.00	0.00	0	126.7510000	-141000.800	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.301121607D+04	-5.858044060D+02	9.322903480D+00	-3.006298824D-03	2.590788666D-06					
-1.080178662D-09	2.341239608D-13							-1.621041276D+04	-1.816752393D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.644123697D+05	6.928002690D+02	4.638270140D+00	2.754339782D-03	-8.624218250D-07					
1.170827576D-10	-5.938061950D-15							-2.219721855D+04	1.116897701D+01

## Appendix D (continued)

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FeCL3                      Chase,1998 p879.
 2 j 6/65 FE 1.00CL 3.00 0.00 0.00 0.00 0 162.2040000 -1059104.288
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18214.073
 4.284772100D+03-5.741705370D+02 1.220667256D+01-4.680434120D-03 5.609500470D-06
-3.549599500D-09 9.198543490D-13 -1.275688456D+05-2.887584081D+01
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18214.073
-5.915740590D+04-1.033382228D+01 1.000849967D+01-3.657651870D-06 8.545873640D-10
-1.023070527D-13 4.904063640D-18 -1.305012050D+05-1.598494171D+01

FeO                      Chase,1998 p1239.
 2 j 9/66 FE 1.000 1.00 0.00 0.00 0.00 0 71.8444000 251040.000
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8837.031
 1.569282213D+04-6.460188880D+01 2.458925470D+00 7.016047360D-03-1.021405947D-05
 7.179297870D-09-1.978966365D-12 2.964572665D+04 1.326115545D+01
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8837.031
-1.195971480D+05-3.624864780D+02 5.518880750D+00-9.978856890D-04 4.376913830D-07
-6.790629460D-11 3.639292680D-15 3.037985806D+04-3.633655420D+00

Fe(OH)2                  Chase,1998 p1230.
 2 j12/66 FE 1.000 2.00H 2.00 0.00 0.00 0 89.8596800 -330536.000
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14209.461
 4.443027200D+05-6.795140890D+03 3.894726210D+01-5.973005680D-02 7.046165430D-05
-4.087859510D-08 9.368766340D-12 -9.051420860D+03-1.931304058D+02
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14209.461
 1.612519190D+06-6.533241990D+03 1.842922816D+01-2.073249635D-03 4.265874360D-07
-4.564063130D-11 1.990105746D-15 -2.992568633D+03-8.445940590D+01

Fe2CL4                  Chase,1998 p891.
 2 j12/70 FE 2.00CL 4.00 0.00 0.00 0.00 0 253.5020000 -431370.400
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29849.201
 1.501308814D+03-6.617096510D+02 1.826924882D+01-4.181494660D-03 4.196535050D-06
-2.188670747D-09 5.395194700D-13 -5.340057580D+04-4.935640680D+01
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29849.201
 1.402450973D+05 6.936064410D+02 1.313800410D+01 2.754333070D-03-8.623996010D-07
 1.170782491D-10-5.937778080D-15 -5.974172730D+04-1.752491511D+01

Fe2CL6                  Chase,1998 p928.
 2 j 6/65 FE 2.00CL 6.00 0.00 0.00 0.00 0 324.4080000 -654377.600
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 40447.854
-1.034544447D+04-8.234876600D+02 2.520090594D+01-6.845796790D-03 8.255820750D-06
-5.248965660D-09 1.365242237D-12 -8.131847190D+04-8.010768938D+01
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 40447.854
-9.999118000D+04-1.457716085D+01 2.201208460D+01-5.229481130D-06 1.226831608D-09
-1.473195806D-13 7.078272330D-18 -8.551496190D+04-6.143757198D+01

Ga                      Hf:Gurvich,1996a. Moore,1971. Johansson,1966. Gordon,1999.
 3 g12/98 GA 1.00 0.00 0.00 0.00 0.00 0 69.7230000 272000.000
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6551.115
 2.387947890D+05-3.121634631D+03 1.630171272D+01-2.347922342D-02 1.932327565D-05
-7.316311870D-09 8.857387735D-13 4.732717380D+04-7.547172760D+01
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6551.115
-5.544186520D+04 8.808624420D+02 1.760717716D+00 2.993259460D-04-5.610827310D-08
 2.682832239D-12 3.132134914D-16 2.684351822D+04 1.252212023D+01
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6551.115
 2.288759836D+08-6.759297920D+04 2.526821493D+00 1.463058875D-03-1.250892936D-07
 3.820116110D-12-3.997883065D-17 6.402915740D+05-8.083504020D+00

Ga+                      IP:Johansson,1966. Moore,1971. Gordon,1999.
 3 g12/98 GA 1.00E -1.00 0.00 0.00 0.00 0 69.7224514 856688.428
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428
 4.098344940D-04-4.343581620D-06 2.500000019D+00-4.389036810D-11 5.563969200D-14
-3.638228260D-17 9.607881995D-21 1.022899726D+05 5.215090460D+00
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428
 3.566607140D+04-1.108845546D+02 2.635517951D+00-8.338973520D-05 2.734243614D-08
-4.555673740D-12 3.035050101D-16 1.029897430D+05 4.257075410D+00
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428
 1.880791061D+08-1.410890480D+05 4.500268850D+01-6.445582900D-03 5.005999840D-07
-1.789454995D-11 2.439723414D-16 1.191428220D+06-3.545671850D+02

GaBr                      Gurvich,1996a pt1 p239 pt2 p193
 2 tpis96 GA 1.00BR 1.00 0.00 0.00 0.00 0 149.6270000 -17967.880
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9932.119
-2.185275415D+03-7.672232970D+01 4.770805670D+00-4.497881060D-04 5.579853600D-07
-3.065156457D-10 7.042946040D-14 -3.138004818D+03 2.948144294D+00
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9932.119
 3.359805030D+05-8.406836680D+02 5.145084730D+00-3.265526000D-05-7.671022750D-08
 3.635123820D-11-3.358177830D-15 2.035179445D+03-4.277894080D-01

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## Appendix D (continued)

GaBr2                      Gurvich,1996a pt1 p241 pt2 p194.

2 tpris96 GA	1.00BR	2.00	0.00	0.00	0.00	0.00	0	229.5310000	-149180.952
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.081681620D+03	-3.705766100D+02	8.418425360D+00	-3.001930915D-03	3.595477670D-06					
-2.276883735D-09	5.913221770D-13			-1.821116655D+04	-9.512572050D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.302294360D+05	4.766722650D+02	7.104725400D+00	-5.522771210D-04	3.159876015D-07					
-5.513637150D-11	3.173293230D-15			-2.365683620D+04	-1.162714892D+00				

GaBr3                      Gurvich,1996a pt1 p243 pt2 p196.

2 tpris96 GA	1.00BR	3.00	0.00	0.00	0.00	0	309.4350000	-292962.663	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.363807340D+03	-5.142040450D+02	1.196065138D+01	-4.134637650D-03	4.933978330D-06					
-3.111868526D-09	8.043631480D-13			-3.570415500D+04	-2.556896053D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.103063750D+04	-9.395209690D+00	1.000768765D+01	-3.295954300D-06	7.679838140D-10					
-9.175147260D-14	4.391186940D-18			-3.833402150D+04	-1.410315914D+01				

GaCL                      Gurvich,1996a pt1 p231 pt2 p186

2 tpris96 GA	1.00CL	1.00	0.00	0.00	0.00	0	105.1760000	-69621.440	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.417143000D+03	-2.257949147D+02	5.311673690D+00	-1.562280975D-03	1.836579731D-06					
-1.100421873D-09	2.725812445D-13			-8.593892330D+03	-1.695911735D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.864842240D+05	1.452870183D+03	2.719542959D+00	1.144285628D-03	3.431452860D-07					
5.470440480D-11	-3.019622103D-15			-1.895084035D+04	1.570926145D+01				

GaCL2                      Gurvich,1996a pt1 p232 pt2 p187.

2 tpris96 GA	1.00CL	2.00	0.00	0.00	0.00	0	140.6290000	-220978.909	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.225481851D+04	-6.046218440D+02	9.220388910D+00	-4.554400790D-03	5.324855180D-06					
-3.308605570D-09	8.462235560D-13			-2.564550386D+04	-1.685409262D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.445405300D+05	4.714437160D+02	7.108775480D+00	-5.539433560D-04	3.163638240D-07					
-5.518023930D-11	3.175353030D-15			-3.230936160D+04	-3.744840740D+00				

GaCL3                      Gurvich,1996a pt1 p235 pt2 p189.

2 tpris96 GA	1.00CL	3.00	0.00	0.00	0.00	0	176.0820000	-432624.753	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.784948400D+04	-1.162678125D+03	1.408954213D+01	-8.106134290D-03	9.219430160D-06					
-5.599710550D-09	1.404852600D-12			-4.915909730D+04	-4.282179383D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.466917310D+04	-2.561468254D+01	1.002010048D+01	-8.354073070D-06	1.901439055D-09					
-2.231168493D-13	1.052949609D-17			-5.518201430D+04	-1.864958383D+01				

GaF                      Gurvich,1996a pt1 p224 pt2 p179

2 tpris96 GA	1.00F	1.00	0.00	0.00	0.00	0	88.7214032	-232608.491	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.670398010D+04	-5.336572220D+02	5.759291920D+00	-1.506128492D-03	9.509038450D-07					
-1.830941130D-10	-3.135959193D-14			-2.647075690D+04	-6.589321880D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.983392279D+05	7.225157870D+02	3.639557430D+00	5.546736760D-04	-1.464901450D-07					
2.177385396D-11	-1.031058874D-15			-3.408528710D+04	7.553960000D+00				

GaF2                      Gurvich,1996a pt1 p225 pt2 p180.

2 tpris96 GA	1.00F	2.00	0.00	0.00	0.00	0	107.7198064	-516712.441	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.842539530D+04	-8.897617740D+02	7.707455490D+00	2.072150890D-03	-5.289981930D-06					
4.564127420D-09	-1.406942753D-12			-5.919856150D+04	-1.341142116D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.100251360D+05	-1.723259472D+03	8.951329220D+00	-1.059205682D-03	2.745755154D-07					
-2.907681311D-11	1.084834142D-15			-5.376571600D+04	-2.113835528D+01				

GaF3                      Gurvich,1996a pt1 p226 pt2 p182.

2 tpris96 GA	1.00F	3.00	0.00	0.00	0.00	0	126.7182096	-921476.983	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.593266700D+04	-1.355507494D+03	1.097760197D+01	3.461571720D-03	-8.469551950D-06					
7.222468930D-09	-2.213328653D-12			-1.061479087D+05	-3.212651850D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.096961760D+05	-1.431211274D+02	1.010568378D+01	-4.184936820D-05	9.164759450D-09					
-1.042661957D-12	4.799163450D-17			-1.136678134D+05	-2.392539330D+01				



## Appendix D (continued)

GaH Gurvich,1996a pt1 p220 pt2 p177  
 2 tps96 GA 1.00H 1.00 0.00 0.00 0.00 0 70.7309400 214323.404  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8673.104  
 -4.391876200D+04 6.254457120D+02 3.276862890D-01 6.496641500D-03-3.802970010D-06  
 2.852103704D-10 3.626809130D-13 2.171260108D+04 2.224032244D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8673.104  
 3.257993990D+06-1.109099502D+04 1.801126796D+01-8.167719110D-03 2.601293566D-06  
 -3.813459350D-10 2.028049649D-14 9.369778240D+04-9.820900220D+01

GaI Gurvich,1996a pt1 p247 pt2 p200  
 2 tps96 GA 1.00I 1.00 0.00 0.00 0.00 0 196.6274700 44871.122  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10109.122  
 -3.661855030D+03-3.206924180D+01 4.599961920D+00-8.899475460D-05 1.162792633D-07  
 -1.812351457D-11-7.584619640D-15 4.198649370D+03 4.928964650D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10109.122  
 1.498356654D+06-4.551967240D+03 9.803005350D+00-2.943735609D-03 8.658040510D-07  
 -1.106638204D-11 5.007836860D-15 3.291811910D+04-3.227359770D+01

GaI2 Gurvich,1996a pt1 p249 pt2 p201.  
 2 tps96 GA 1.00I 2.00 0.00 0.00 0.00 0 323.5319400 -28954.965  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14470.935  
 -9.831395900D+02-2.152621259D+02 7.844318760D+00-1.819797849D-03 2.210706958D-06  
 -1.416110855D-09 3.713762930D-13 -4.534090230D+03-4.250516810D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14470.935  
 -3.202879750D+05 4.796502330D+02 7.102333960D+00-5.512657830D-04 3.157543452D-07  
 -5.510871940D-11 3.171977730D-15 -9.180919610D+03 7.275204880D-01

GaI3 Gurvich,1996a pt1 p250 pt2 p203.  
 2 tps96 GA 1.00I 3.00 0.00 0.00 0.00 0 450.4364100 -115877.240  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20122.760  
 -5.663472650D+03-2.425937116D+02 1.095451119D+01-2.059175489D-03 2.499117622D-06  
 -1.596502506D-09 4.167644060D-13 -1.576722832D+04-1.646129942D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20122.760  
 -3.164040130D+04-4.208662830D+00 1.000352001D+01-1.532650180D-06 3.611531540D-10  
 -4.350978870D-14 2.095704875D-18 -1.700058453D+04-1.090291552D+01

GaO Gurvich,1996a pt1 p214 pt2 p174  
 2 tps96 GA 1.00O 1.00 0.00 0.00 0.00 0 85.7224000 146823.607  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8925.107  
 7.325543910D+04-9.804269510D+02 7.844122760D+00-7.171072850D-03 7.872780510D-06  
 -2.401464112D-09-2.594919458D-13 2.140581724D+04-1.799742951D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8925.107  
 2.937313804D+06-1.118314112D+04 1.859366773D+01-6.854753450D-03 1.665399251D-06  
 -1.887560878D-10 7.972686920D-15 8.530248080D+04-9.904040480D+01

GaOH Gurvich,1996a pt1 p222 pt2 p178.  
 2 tps96 GA 1.00O 1.00H 1.00 0.00 0.00 0 86.7303400 -143630.495  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10583.608  
 6.963101870D+04-1.247828695D+03 1.022001611D+01-5.922534390D-03 4.643387400D-06  
 -1.215936978D-09-2.945243614D-14 -1.275397794D+04-3.217063000D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10583.608  
 8.429051010D+05-2.372324595D+03 8.009071090D+00 8.777230710D-05-5.943068910D-08  
 9.841943440D-12-5.531552790D-16 -3.751788250D+03-2.171053719D+01

Ga2Br2 Gurvich,1996a pt1 p244 pt2 p197.  
 2 tps96 GA 2.00BR 2.00 0.00 0.00 0.00 0 299.2540000 -136963.692  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20793.308  
 -1.117183241D+04-7.471471620D+01 1.030246084D+01-6.657929850D-04 8.200515850D-07  
 -5.297021520D-10 1.394553192D-13 -1.913297856D+04-1.317110316D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20793.308  
 -1.885373131D+04-1.263621802D+00 1.000108034D+01-4.774975660D-07 1.137227648D-10  
 -1.380820486D-14 6.690242430D-19 -1.951053843D+04-1.141667594D+01

Ga2Br4 Gurvich,1996a pt1 p245 pt2 p198.  
 2 tps96 GA 2.00BR 4.00 0.00 0.00 0.00 0 459.0620000 -415820.034  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 30591.766  
 -1.315545939D+04-4.136553020D+02 1.762849229D+01-3.514652160D-03 4.266937730D-06  
 -2.726515882D-09 7.118924490D-13 -5.283101810D+04-4.427520690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 30591.766  
 -5.742167210D+04-7.160137370D+00 1.600598947D+01-2.608182270D-06 6.146455950D-10  
 -7.405438650D-14 3.567126630D-18 -5.493389760D+04-3.479271660D+01

## Appendix D (continued)

Ga2Br6                      Gurvich,1996a pt1 p246 pt2 p199.

2 tps96 GA	2.00BR	6.00	0.00	0.00	0.00	0	618.8700000	-673688.732
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-6.725116890D+03	-8.067526550D+02	2.511671424D+01	-6.636514570D-03	7.977555700D-06				
-5.059685210D-09	1.313546388D-12		-8.370635200D+04	-7.585278720D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-9.526173000D+04	-1.444681880D+01	2.201192546D+01	-5.145006740D-06	1.204348449D-09				
-1.443806473D-13	6.928270740D-18		-8.782223300D+04	-5.765895120D+01				

Ga2CL2                      Gurvich,1996a pt1 p237 pt2 p190.

2 tps96 GA	2.00CL	2.00	0.00	0.00	0.00	0	210.3520000	-220972.686
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-9.246133700D+03	-2.592159934D+02	1.102847129D+01	-2.231983927D-03	2.720723456D-06				
-1.743798624D-09	4.563666040D-13		-2.834059821D+04	-2.067773272D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-3.668954200D+04	-4.434580680D+00	1.000373051D+01	-1.630793333D-06	3.853753320D-10				
-4.652527730D-14	2.244498791D-18		-2.965633085D+04	-1.469535817D+01				

Ga2CL4                      Gurvich,1996a pt1 p237 pt2 p191.

2 tps96 GA	2.00CL	4.00	0.00	0.00	0.00	0	281.2580000	-602326.828
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
1.637343702D+04	-1.140637354D+03	2.030139827D+01	-8.997746200D-03	1.067254867D-05				
-6.700290620D-09	1.725749144D-12		-7.162385010D+04	-6.666361900D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-1.127110409D+05	-2.138517542D+01	1.601738077D+01	-7.415564640D-06	1.721694751D-09				
-2.051361953D-13	9.797311500D-18		-7.746853380D+04	-4.147280870D+01				

Ga2CL6                      Gurvich,1996a pt1 p238 pt2 p192.

2 tps96 GA	2.00CL	6.00	0.00	0.00	0.00	0	352.1640000	-962463.532
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
6.089469840D+04	-2.104456302D+03	2.959653878D+01	-1.537809796D-02	1.779096808D-05				
-1.095619429D-08	2.779706493D-12		-1.118400535D+05	-1.121945814D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-1.898445426D+05	-4.413655240D+01	2.203505047D+01	-1.470071128D-05	3.369512810D-09				
-3.975462800D-13	1.884231868D-17		-1.226969998D+05	-6.745332883D+01				

Ga2F2                      Gurvich,1996a pt1 p228 pt2 p183.

2 tps96 GA	2.00F	2.00	0.00	0.00	0.00	0	177.4428064	-606231.344
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
2.978130650D+04	-1.013975520D+03	1.374933053D+01	-7.728050960D-03	9.064007330D-06				
-5.641193220D-09	1.443106716D-12		-7.086083370D+04	-4.109833950D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-8.773234930D+04	-1.983775870D+01	1.001594030D+01	-6.744402830D-06	1.556129063D-09				
-1.845316975D-13	8.780884020D-18		-7.607368630D+04	-1.908325521D+01				

Ga2F4                      Gurvich,1996a pt1 p228 pt2 p184.

2 tps96 GA	2.00F	4.00	0.00	0.00	0.00	0	215.4396128	-1325002.958
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
1.422079998D+05	-2.798829941D+03	2.395904235D+01	-1.293904774D-02	1.223101326D-05				
-6.251209820D-09	1.334919195D-12		-1.496013710D+05	-9.734153640D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-2.704366090D+05	-1.049957196D+02	1.607903965D+01	-3.178895920D-05	7.049582720D-09				
-8.102379520D-13	3.760540530D-17		-1.644169589D+05	-4.896591730D+01				

Ga2F6                      Gurvich,1996a pt1 p230 pt2 p185.

2 tps96 GA	2.00F	6.00	0.00	0.00	0.00	0	253.4364192	-2017623.843
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
2.409045572D+05	-4.142379800D+03	3.195773720D+01	-1.297914290D-02	8.959282190D-06				
-2.733621068D-09	1.554030994D-13		-2.272785240D+05	-1.398403732D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-4.368664800D+05	-2.128208368D+02	2.215886373D+01	-6.346287910D-05	1.399738556D-08				
-1.601732039D-12	7.407584420D-17		-2.494298707D+05	-7.787635830D+01				

Ga2I2                      Gurvich,1996a pt1 p252 pt2 p204.

2 tps96 GA	2.00I	2.00	0.00	0.00	0.00	0	393.2549400	13520.947
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-8.960252670D+03	-3.172057210D+01	1.012930491D+01	-2.860191165D-04	3.535333010D-07				
-2.289632389D-10	6.040085360D-14		-1.233174068D+03	-9.801968380D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								0.0
-1.219056501D+04	-5.287554470D-01	1.000045392D+01	-2.011599344D-07	4.799467810D-11				
-5.834781080D-15	2.829565069D-19		-1.393258606D+03	-9.052614910D+00				

## Appendix D (continued)

Ga2I4                      Gurvich,1996a pt1 p253 pt2 p205.

2 tpi96 GA	2.00I	4.00	0.00	0.00	0.00	0.00	0	647.0638800	-159267.987
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.769495991D+04	-1.354871509D+02	1.654625333D+01	-1.199014713D-03	1.473754848D-06					
-9.504796570D-10	2.499380837D-13		-2.333405795D+04	-3.325712890D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									32583.813
-3.171299760D+04	-2.287068836D+00	1.600194812D+01	-8.588964380D-07	2.041966602D-10					
-2.476145769D-14	1.198551944D-18		-2.401940505D+04	-3.008672521D+01					

Ga2I6                      Gurvich,1996a pt1 p253 pt2 p206.

2 tpi96 GA	2.00I	6.00	0.00	0.00	0.00	0	900.8728200	-317294.623	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.110891458D+04	-3.695404160D+02	2.346811836D+01	-3.189178210D-03	3.890339040D-06					
-2.494830378D-09	6.532007280D-13		-4.301188090D+04	-6.014811500D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									43573.378
-6.015698150D+04	-6.329209230D+00	2.200533040D+01	-2.332008629D-06	5.513868480D-10					
-6.659445350D-13	3.213670430D-18		-4.488699380D+04	-5.161008750D+01					

Ga2O                      Gurvich,1996a pt1 p216 pt2 p175.

2 tpi96 GA	2.00I	1.00	0.00	0.00	0.00	0	155.4454000	-99457.457	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.697197180D+04	-8.074085990D+02	7.733061540D+00	1.478450874D-03	-4.097743430D-06					
3.581158920D-09	-1.107073202D-12		-9.512216820D+03	-1.256149299D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									12162.595
-1.193874986D+05	-8.719341610D+01	7.064678200D+00	-2.571524542D-05	5.651108490D-09					
-6.448190540D-13	2.975374645D-17		-1.393694796D+04	-6.942801300D+00					

Ge                      Hf:Gurvich,1991 pt1 p311. Sugar,1993. Gordon,1999.

3 g 3/99 GE	1.00	0.00	0.00	0.00	0.00	0	72.6400000	367800.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.059215242D+04	-1.432022103D+02	4.506002330D+00	1.547187840D-03	-8.518296550D-06					
8.243824460D-09	-2.566167305D-12		4.363070860D+04	-6.224648889D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									7398.584
-8.565413840D+05	3.917958660D+03	-1.809888212D+00	2.276482224D-03	-5.365627550D-07					
5.984958090D-11	-2.541700646D-15		1.956518798D+04	3.841408752D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									7398.584
2.423965136D+07	-2.543605174D+04	1.456087539D+01	-2.592562254D-03	2.658628502D-07					
-1.122785077D-11	1.620997559D-16		2.295812461D+05	-8.953523898D+01					

Ge+                      Sugar,1993. Gordon,1999.

3 g 3/99 GE	1.00E	-1.00	0.00	0.00	0.00	0	72.6394514	1134984.385	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.453666430D+05	4.008449710D+03	-1.522395737D+01	3.626030020D-02	-3.351367260D-05					
1.431059219D-08	-2.236976459D-12		1.157058042D+05	1.090158182D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6205.785
-2.244860570D+06	5.165531140D+03	-3.867516510D-01	8.528730940D-04	-1.386040003D-07					
1.155945775D-11	-3.784413134D-16		1.006823985D+05	2.965845411D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6205.785
5.768056240D+07	-3.078606210D+04	8.706291820D+00	-4.942233500D-04	-2.690467703D-11					
1.853441677D-12	-5.082067525D-17		3.857785420D+05	-4.842537137D+01					

Ge-                      Hotop,1985. Gordon,1999.

3 g 3/99 GE	1.00E	1.00	0.00	0.00	0.00	0	72.6405486	245402.540	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.989142308D+03	8.657417230D+01	2.191868507D+00	5.900795270D-04	-6.375800580D-07					
3.661132150D-10	-8.689778450D-14		2.835695190D+04	9.417623637D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6980.940
1.352040246D+04	-5.048518780D-01	2.500140247D+00	-3.652944160D-09	-6.716722200D-12					
1.378119925D-15	-8.475212940D-20		2.881739757D+04	7.577953867D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									6980.940
1.079877187D+04	1.149969180D+00	2.499738027D+00	3.051383052D-08	-1.930296476D-12					
6.305166240D-17	-8.327676240D-22		2.880429709D+04	7.581467327D+00					

GeBr                      Gurvich,1991 pt1 p333 pt2 p287.

2 tpi91 GE	1.00BR	1.00	0.00	0.00	0.00	0	152.5440000	137438.119	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.680774630D+04	9.173361260D+02	-2.224809366D+00	2.171239242D-02	-3.035490868D-05					
2.011776305D-08	-5.202915040D-12		1.104192901D+04	4.107865983D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									9864.119
2.256750476D+05	-7.310715460D+02	6.263283810D+00	-1.198085447D-03	4.000377770D-07					
-5.429937880D-11	2.510481953D-15		1.942863606D+04	-6.106507844D+00					

## Appendix D (continued)

GeBr2 Gurvich,1991 pt1 p334 pt2 p288.

2 tps91 GE	1.00BR	2.00	0.00	0.00	0.00	0.00	0	232.4480000	-60962.897
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.649285325D+03	-2.296262116D+02	7.900144680D+00	-1.936685504D-03	2.345776175D-06					
-1.496279368D-09	3.901453500D-13		-8.316624210D+03	-6.918156136D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.636655245D+04	-3.990509020D+00	7.003327440D+00	-1.445749787D-06	3.401591360D-10					
-4.093457030D-14	1.969987842D-18		-9.484999250D+03	-1.673617098D+00					

GeBr3 Gurvich,1991 pt1 p335 pt2 p289.

2 tps91 GE	1.00BR	3.00	0.00	0.00	0.00	0	312.3520000	-119031.308	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.725568677D+03	-5.186213260D+02	1.199957754D+01	-4.251024530D-03	5.103629720D-06					
-3.233706250D-09	8.388358860D-13		-1.477988251D+04	-2.534555678D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.433926700D+04	-9.280327950D+00	1.000765019D+01	-3.297322150D-06	7.712929260D-10					
-9.241571850D-14	4.432876230D-18		-1.742697092D+04	-1.366946296D+01					

GeBr4 Gurvich,1991 pt1 p336 pt2 p290.

2 tps91 GE	1.00BR	4.00	0.00	0.00	0.00	0	392.2560000	-291000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.431940390D+03	-6.777748800D+02	1.560015305D+01	-5.507788880D-03	6.594764290D-06					
-4.170146140D-09	1.080116643D-12		-3.557606400D+04	-4.209122927D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.977757910D+04	-1.179873115D+01	1.300953955D+01	-4.024938750D-06	9.203567210D-10					
-1.076853369D-13	5.040954800D-18		-3.904148160D+04	-2.689436070D+01					

GeCL Gurvich,1991 pt1 p328 pt2 p283.

2 tps91 GE	1.00CL	1.00	0.00	0.00	0.00	0	108.0930000	69029.915	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.069724739D+04	-2.241238266D+01	1.987371070D+00	1.368270905D-02	-2.358294414D-05					
1.786756020D-08	-5.102503250D-12		7.440683390D+03	1.505837189D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.784193250D+05	1.429309204D+03	3.194854640D+00	8.119939120D-04	-2.652459954D-07					
5.151957880D-11	-3.534214570D-15		-2.087046335D+03	1.385033820D+01					

GeCL2 Gurvich,1991 pt1 p330 pt2 p284.

2 tps91 GE	1.00CL	2.00	0.00	0.00	0.00	0	143.5460000	-171000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.838536673D+04	-5.827205340D+02	9.161404660D+00	-4.464786030D-03	5.244873550D-06					
-3.268067210D-09	8.367575420D-13		-1.975798598D+04	-1.734321630D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.890128920D+04	-1.126210418D+01	7.009063530D+00	-3.839180730D-06	8.865633570D-10					
-1.052000540D-13	5.008422220D-18		-2.275254424D+04	-4.656641298D+00					

GeCL3 Hf:Gurvich,1991 pt1 p331. Gurvich,1979 pt2 p287.

2 g 6/01 GE	1.00CL	3.00	0.00	0.00	0.00	0	178.9990000	-266950.589	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.935859579D+04	-8.342020000D+02	1.312702530D+01	-6.511390020D-03	7.696277480D-06					
-4.818541730D-09	1.238399959D-12		-3.097218753D+04	-3.552547184D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.574499820D+04	-1.579213420D+01	1.001278835D+01	-5.441738310D-06	1.260936724D-09					
-1.500137106D-13	7.156400810D-18		-3.525131720D+04	-1.719719944D+01					

GeCL4 Gurvich,1991 pt1 p332 pt2 p286.

2 tps91 GE	1.00CL	4.00	0.00	0.00	0.00	0	214.4520000	-500000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.502870410D+04	-1.652482760D+03	1.881327000D+01	-1.152426810D-02	1.310809980D-05					
-7.961956110D-09	1.997505040D-12		-5.570052390D+04	-6.754438135D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.376261210D+05	-3.603769500D+01	1.302816670D+01	-1.164956960D-05	2.636193380D-09					
-3.072926720D-13	1.439808750D-17		-6.426281780D+04	-3.318158305D+01					

GeF Gurvich,1991 pt1 p324 pt2 p279.

2 tps91 GE	1.00F	1.00	0.00	0.00	0.00	0	91.6384032	-70592.990	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.017097820D+04	-4.395552520D+02	2.990864513D+00	1.252766738D-02	-2.337593226D-05					
1.841631179D-08	-5.398492260D-12		-7.093516400D+03	7.064248931D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.150480580D+05	1.659711777D+03	2.999610299D+00	8.198511680D-04	-2.271982948D-07					
3.624183860D-11	-2.133840473D-15		-2.051529487D+04	1.373154230D+01					

## Appendix D (continued)

GeF2                      Gurvich,1991 pt1 p326 pt2 p280.

2	tpis91	GE	1.00F	2.00	0.00	0.00	0.00	0	110.6368064	-574000.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
7.543097080D+04	-1.108456469D+03	9.078898270D+00	-1.445630636D-03	-6.575322320D-07						
1.475344103D-09	-5.811220270D-13		-6.510685550D+04	-2.200457134D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11787.485
-1.275327716D+05	-7.162591350D+01	7.053002370D+00	-2.101910441D-05	4.607893700D-09						
-5.246394670D-13	2.416218951D-17		-7.112637630D+04	-8.483841439D+00						

GeF3                      Hf:Gurvich,1991 pt1 p327. Gurvich,1979 v2 pt2 p283.

2	g	6/01	GE	1.00F	3.00	0.00	0.00	0	129.6352096	-806332.833
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
1.114121569D+05	-1.776908030D+03	1.352166477D+01	-2.983622949D-03	-3.612749750D-08						
1.621528436D-09	-7.199011780D-13		-9.038262960D+04	-4.568760023D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	14678.187
-2.069580129D+05	-1.110233803D+02	1.008234122D+01	-3.271676260D-05	7.183896700D-09						
-8.190388120D-13	3.776322440D-17		-9.999749090D+04	-2.303465940D+01						

GeF4                      Gurvich,1991 pt1 p328 pt2 p282.

2	tpis91	GE	1.00F	4.00	0.00	0.00	0.00	0	148.6336128	-1190150.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
1.119818968D+05	-1.636859630D+03	1.231371005D+01	1.025446325D-02	-1.893783072D-05						
1.476849261D-08	-4.325174110D-12		-1.374265128D+05	-4.104202391D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17293.025
-3.253032680D+05	-2.538279448D+02	1.318792173D+01	-7.460058550D-05	1.637384721D-08						
-1.866482733D-12	8.605530500D-17		-1.466176526D+05	-4.122237561D+01						

GeH4                      Barin,1989 pt1 p628.

2	bar89	GE	1.00H	4.00	0.00	0.00	0.00	0	76.6717600	90793.000
298.150	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.568398191D+05	-4.132811450D+01	7.755116280D+00	2.129640783D-03	7.255053610D-07						
-5.096314010D-10	1.431608261D-13		7.881538040D+03	-2.030107999D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	0.000
-3.809805880D+06	1.093167093D+04	-5.149675410D+00	9.485931370D-03	-1.649459859D-06						
1.419674126D-10	-5.004639750D-15		-6.158518520D+04	7.168961273D+01						

GeI                      Gurvich,1991 pt1 p337 pt2 p291.

2	tpis91	GE	1.00I	1.00	0.00	0.00	0.00	0	199.5444700	210969.120
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.438308220D+04	1.033759595D+03	-1.520491112D+00	1.555125152D-02	-1.683415215D-05						
8.383557810D-09	-1.550875391D-12		1.912920413D+04	3.959395473D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10005.120
-2.133148437D+05	-2.953079008D+02	6.876607360D+00	-2.102579132D-03	8.596299380D-07						
-1.447692760D-10	8.401042790D-15		2.452326136D+04	-8.549783749D+00						

GeO                      Gurvich,1991 pt1 p315 pt2 p274.

2	tpis91	GE	1.00O	1.00	0.00	0.00	0.00	0	88.6394000	-37694.307
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.781225630D+03	2.791946972D+02	6.198952860D-01	1.111378013D-02	-1.501027092D-05						
1.006783003D-08	-2.687101932D-12		-6.711847430D+03	2.156441027D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8782.106
-1.044508485D+06	2.734866048D+03	1.298071298D+00	1.832638634D-03	-5.060986350D-07						
6.374958020D-11	-2.172371872D-15		-2.362104658D+04	2.350906051D+01						

GeO2                      Gurvich,1991 pt1 p323 pt2 p278.

2	tpis91	GE	1.00O	2.00	0.00	0.00	0.00	0	104.6388000	-106171.998
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.824173830D+03	1.563451633D+02	1.694198285D+00	1.756205059D-02	-2.418270032D-05						
1.632388154D-08	-4.368957860D-12		-1.477534880D+04	1.556926515D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	11258.002
-1.727347526D+05	-2.961154443D+02	7.720726250D+00	-8.824933390D-05	1.949874702D-08						
-2.235834829D-12	1.036128507D-16		-1.387983288D+04	-1.669845695D+01						

GeS                      Gurvich,1991 pt1 p344 pt2 p297.

2	tpis91	GE	1.00S	1.00	0.00	0.00	0.00	0	104.7050000	92525.110
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
3.661018430D+04	-5.659653500D+02	6.152936410D+00	-2.746908039D-03	2.733435196D-06						
-1.460209187D-09	3.278709470D-13		1.274175754D+04	-7.705659460D+00						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9141.110
-2.351367441D+06	7.211581860D+03	-4.362526310D+00	5.451737750D-03	-1.721002774D-06						
2.632908084D-10	-1.394374040D-14		-3.583317250D+04	6.505566891D+01						

## Appendix D (continued)

GeS2                      Gurvich,1991 pt1 p347 pt2 p299.

2 tpis91 GE	1.00S	2.00	0.00	0.00	0.00	0.00	0	136.7700000	118817.831
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.543683600D+04	-1.024826697D+03	1.057594552D+01	-5.287883910D-03	5.295803080D-06					
-2.872529530D-09	6.519027550D-13				1.735579668D+04	-2.991719536D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.970980360D+04	-3.364377000D+01	7.525433720D+00	-1.026368137D-05	2.282230718D-09					
-2.628748770D-13	1.222218614D-17				1.195232103D+04	-1.135170616D+01			

Ge2                      Gurvich,1991 pt1 p313 pt2 p273.

2 tpis91 GE	2.00	0.00	0.00	0.00	0.00	0	145.2800000	471498.929	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.161978929D+05	-3.079621733D+03	1.888047728D+01	-2.604825861D-02	2.279151350D-05					
-9.028351270D-09	1.146806387D-12				7.032402550D+04	-7.901095968D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.969461258D+06	-5.248687100D+03	1.058277303D+01	-3.336551510D-03	1.052745838D-06					
-1.484534793D-10	7.475431760D-15				8.925665990D+04	-3.750233948D+01			

H                      D0(H2):Herzberg,1970. Moore,1972. Gordon,1999.

3 g 6/97 H	1.00	0.00	0.00	0.00	0.00	0	1.0079400	217998.828	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				2.547370801D+04	-4.466828530D-01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.078774250D+01	-1.819354417D-01	2.500211817D+00	-1.226512864D-07	3.732876330D-11					
-5.687744560D-15	3.410210197D-19				2.547486398D+04	-4.481917770D-01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.173757694D+08	-1.312035403D+05	3.399174200D+01	-3.813999680D-03	2.432854837D-07					
-7.694275540D-12	9.644105630D-17				1.067638086D+06	-2.742301051D+02			

H+                      IP(H): Moore,1972. Gordon,1999.

3 g10/00 H	1.00E	-1.00	0.00	0.00	0.00	0	1.0073914	1536245.928	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				1.840214877D+05	-1.140646644D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				1.840214877D+05	-1.140646644D+00			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				1.840214877D+05	-1.140646644D+00			

H-                      Hotop,1985. Gordon,1999.

3 g 9/96 H	1.00E	1.00	0.00	0.00	0.00	0	1.0084886	139031.328	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				1.597615494D+04	-1.139013868D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				1.597615494D+04	-1.139013868D+00			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00				1.597615494D+04	-1.139013868D+00			

HALO                      Gurvich,1996a pt1 p147 pt2 p111.

2 tpis96 AL	1.000	1.00H	1.00	0.00	0.00	0	43.9888780	1821.114	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.668671568D+04	-4.663214590D+02	5.383800210D+00	2.902425002D-03	-2.243677610D-07					
-1.516294323D-09	6.951737660D-13				1.235914473D+03	-6.508837520D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.847467050D+04	-1.515628850D+03	8.572776230D+00	-4.142611440D-04	8.935081700D-08					
-1.007036446D-11	4.608017250D-16				6.663241890D+03	-2.672948642D+01			

HALO2                      Gurvich,1996a pt1 p148 pt2 p112.

2 tpis96 H	1.00AL	1.000	2.00	0.00	0.00	0	59.9882780	-355473.551	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.544598910D+03	1.159819104D+02	8.637970690D-01	2.460875785D-02	-3.423160120D-05					
2.373182987D-08	-6.467608830D-12				-4.449506140D+04	2.012317065D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.985705440D+05	-2.864935042D+03	1.086721494D+01	-5.368312700D-05	-2.836877559D-08					
6.291641190D-12	-3.889033110D-16				-2.764392495D+04	-3.775886340D+01			

## Appendix D (continued)

HBO Boron oxide-hydride Gurvich,1996 pt1 p39,pt2 p23.

2 tps96 H	1.00B	1.000	1.00	0.00	0.00	0	27.8183400	-210621.205
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.360975030D+04	-8.001557590D+02	6.218816130D+00	-7.801679980D-04	3.141286759D-06				
-2.031853478D-09	3.738552890D-13		-2.240282910D+04	-1.326952393D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.861860230D+05	-3.913068050D+03	9.888644800D+00	-8.222269140D-04	1.621530554D-07				
-1.703550237D-11	7.372740020D-16		-3.161852029D+03	-4.036812720D+01				

HBO+ Chase,1998 p223 12/75.

3 g 1/01 H	1.00B	1.000	1.00E	-1.00	0.00	0	27.8177914	1175219.729
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.524471470D+04	7.047337360D+02	5.294271870D+00	1.308494598D-03	2.088343622D-06				
-2.564100339D-09	8.198981250D-13		1.439293436D+05	-6.816749230D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.836083606D+04	-1.212975446D+03	6.822901960D+00	9.142272500D-04	-2.665355457D-07				
3.297049810D-11	-1.530684082D-15		1.463617504D+05	-1.699646159D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.428406068D+07	1.188114816D+04	5.641928570D+00	1.354130653D-04	-2.943428505D-09				
-3.120357467D-14	1.432576207D-18		3.883449210D+04	-3.069802126D+00				

HBO2 Gurvich,1996a pt1 p42 pt2 p26.

2 tps96 H	1.00B	1.000	2.00	0.00	0.00	0	43.8177400	-560210.053
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.225087470D+03	7.566153690D+01	1.253406833D+00	1.748006535D-02	-1.982688351D-05				
1.229656460D-08	-3.153609847D-12		-6.878588780D+04	1.767793507D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.049369185D+06	-4.479145480D+03	1.197755861D+01	-4.735743400D-04	6.080207140D-08				
-3.641565440D-12	6.155973170D-17		-4.221149470D+04	-4.911366820D+01				

HBS Chase,1998 p227 12/75. Jacox,1994.

2 g 2/01 H	1.00B	1.00S	1.00	0.00	0.00	0	43.8839400	50208.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.649966210D+04	-5.466409950D+02	3.636458390D+00	9.963657670D-03	-1.395090386D-05				
1.032834167D-08	-3.047186722D-12		7.919860530D+03	1.182455314D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.021836183D+05	-5.052026620D+02	6.415218280D+00	1.049432932D-03	-3.683146690D-07				
5.342968310D-11	-2.154140451D-15		6.485475620D+03	-1.331379864D+01				

HBS+ Chase,1998 p228 12/75. Jacox,1998 p141.

3 g 1/01 H	1.00B	1.00S	1.00E	-1.00	0.00	0	43.8833914	1129458.967
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.489509163D+05	-1.847661736D+03	1.147458020D+01	-9.476828370D-03	1.110746739D-05				
-6.175558610D-09	1.336853512D-12		1.437822395D+05	-4.113512498D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.610658360D+05	-2.791498527D+03	9.131267640D+00	-5.063795290D-04	7.751213140D-08				
-4.191132930D-12	2.687149095D-17		1.510734114D+05	-3.081426166D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.547637920D+06	7.401763110D+03	4.866419360D+00	4.143886550D-04	-2.488064459D-08				
6.972990680D-13	-7.714953540D-18		7.555300990D+04	3.822638009D+00				

HBr Gurvich,1989 pt1 p205 pt2 p106.

2 tps89 H	1.00BR	1.00	0.00	0.00	0.00	0	80.9119400	-36290.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.527222498D+04	-4.065110270D+02	6.043116610D+00	-7.717882870D-03	1.149123213D-05				
-7.293633280D-09	1.747406491D-12		-3.510414550D+03	-9.903186290D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.170033949D+06	-3.786521010D+03	7.503148050D+00	-1.284963943D-03	3.206257190D-07				
-3.444925160D-11	1.126758417D-15		1.856413349D+04	-2.562712911D+01				

HCN Hf: East,1993. Gurvich,1991 pt1 p226.

2 g 6/01 H	1.00C	1.00N	1.00	0.00	0.00	0	27.0253400	133082.460
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.098286930D+04	-1.238657512D+03	8.721307870D+00	-6.528242940D-03	8.872700830D-06				
-4.808886670D-09	9.317898500D-13		2.098915450D+04	-2.746678076D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.236889278D+06	-4.446732410D+03	9.738874850D+00	-5.855182640D-04	1.072791440D-07				
-1.013313244D-11	3.348247980D-16		4.221513770D+04	-4.005774072D+01				

HCO Hf:Terentis,1996. Jacox,1998 p146.

2 g 1/01 H	1.00C	1.00O	1.00	0.00	0.00	0	29.0180400	42397.850
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.189851887D+04	2.151536111D+02	2.730224028D+00	1.806516108D-03	4.984300570D-06				
-5.814567920D-09	1.869689894D-12		2.905755640D+03	1.136772540D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.949606120D+05	-3.656223380D+03	9.604731170D+00	-1.117129278D-03	2.875328019D-07				
-3.626247740D-11	1.808329595D-15		2.543704440D+04	-3.582473720D+01				

## Appendix D (continued)

HCO+                      Formyl ion. Hf:Chase,1998 p603 12/70. Jacox,1998 p145.

3 g 1/01 H	1.00C	1.000	1.00E	-1.00	0.00	0	29.0174914	833034.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.573442506D+05	-1.867692159D+03	1.099235423D+01	-1.211637888D-02	1.659091514D-05				
-1.016592642D-08	2.391234771D-12		1.084930280D+05	-4.078261620D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.219060653D+06	-4.714294890D+03	1.021192493D+01	-8.854517070D-04	1.667408026D-07				
-1.683285548D-11	7.040051780D-16		1.277989027D+05	-4.351158460D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.593151930D+05	-1.132568857D+03	7.739065200D+00	-2.648464060D-05	1.613280824D-09				
-5.113217500D-14	6.588027500D-19		1.032813937D+05	-2.458716820D+01				

HCCN                      Gurvich,1989 pt1 p228 pt2 p216.

2 tpis89 H	1.00C	2.00N	1.00	0.00	0.00	0	39.0360400	610430.628
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.994114377D+03	-4.404660680D+02	6.940036410D+00	3.846304960D-03	-1.264728529D-06				
-3.639235130D-10	2.748929104D-13		7.370878640D+04	-1.315302591D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.395620310D+05	-4.091067750D+03	1.272233302D+01	-6.8744405310D-04	1.231169968D-07				
-1.186956238D-11	4.760610350D-16		9.585164820D+04	-5.248695794D+01				

HCCO                      Ketenyl rad. Osborn,1997. Szalay,1996. Jacox,1998 p156.

2 g 6/01 H	1.00C	2.00O	1.00	0.00	0.00	0	41.0287400	176568.100
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.959612700D+04	-1.164594402D+03	9.456616260D+00	-2.331240632D-03	5.161873600D-06				
-3.526169970D-09	8.599143230D-13		2.535003992D+04	-2.72635531D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.093922002D+06	-4.498228210D+03	1.246446433D+01	-6.343317400D-04	1.108549019D-07				
-1.125488678D-11	5.689151940D-16		4.652280300D+04	-5.099070430D+01				

HCL                      Gurvich,1989 pt1 p186 pt2 p93.

2 tpis89 H	1.00CL	1.00	0.00	0.00	0.00	0	36.4609400	-92310.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.062588287D+04	-3.093368855D+02	5.275418850D+00	-4.828874220D-03	6.195794600D-06				
-3.040023782D-09	4.916790030D-13		-1.067782299D+04	-7.309305408D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.157749510D+05	-2.770550211D+03	5.973539790D+00	-3.629810060D-04	4.735529190D-08				
2.810262054D-12	-6.656104220D-16		5.674958050D+03	-1.642825822D+01				

HD                      Gurvich,1989 pt1 p144 pt2 p53.

3 tpis89 H	1.00D	1.00	0.00	0.00	0.00	0	3.0220420	323.302
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.519120338D+04	-2.761004999D+02	4.644441290D+00	-2.082376844D-03	1.418070803D-06				
2.839893835D-10	3.202331030D-13		3.913616430D+02	-9.395396120D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.455830000D+05	-1.956578537D+03	4.404373870D+00	5.751681090D-04	-2.131983152D-07				
4.036126680D-11	-2.727170705D-15		1.227254163D+04	-1.084742878D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.829960940D+08	-3.077144916D+05	7.864816510D+01	-8.332990910D-03	4.732254110D-07				
-1.372721571D-11	1.614120677D-16		2.431070386D+06	-6.569437060D+02				

HD+                      Chase,1998 p1034.

3 j 9/77 H	1.00D	1.00E	-1.00	0.00	0.00	0	3.0214934	1496792.618
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.070073050D+04	8.796432580D+02	5.968932160D-02	5.418181010D-03	-2.021515155D-06				
-4.945261650D-10	4.092935650D-13		1.744992497D+05	1.934281193D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.340083030D+06	-5.730069570D+03	1.213836576D+01	-5.243338120D-03	1.976302344D-06				
-3.306573530D-10	1.937902763D-14		2.135348051D+05	-6.128758390D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.116880040D+06	-1.884939608D+04	1.741572175D+01	-2.495631471D-03	1.746560021D-07				
-5.815870420D-12	7.638706130D-17		3.018292196D+05	-1.105093671D+02				

HDO                      Gurvich,1989 pt1 p145 pt2 p55.

2 g 5/99 H	1.00D	1.00O	1.00	0.00	0.00	0	19.0214420	-245280.477
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.737795356D+04	4.310503900D+02	1.558479899D+00	5.764969150D-03	-4.855129360D-06				
3.382990170D-09	-1.040863879D-12		-3.273226450D+04	1.487751891D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.711376798D+06	-5.322872300D+03	9.124351520D+00	-3.400664150D-04	4.152343520D-08				
-4.780768570D-14	-1.468035170D-16		3.245224680D+03	-3.774600680D+01				



## Appendix D (continued)

HDO2                      Gurvich,1989 pt1 p146 pt2 p56.

2 g	5/99 H	1.00D	1.000	2.00	0.00	0.00	0	35.0208420	-140241.635
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
									11334.965

-3.216476650D+04 7.492334460D+02-1.957676212D+00 2.412802791D-02-2.915946684D-05  
1.930016324D-08-5.226986310D-12 -2.151059175D+04 3.672406740D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11334.965  
1.313180619D+06-5.175637120D+03 1.216490975D+01-6.136699480D-04 1.227560176D-07  
-1.079624939D-11 3.874013720D-16 1.303209670D+04-5.085276870D+01

HF                      Gurvich,1989 pt1 p162 pt2 p77.

3 tpis89 H	1.00F	1.00	0.00	0.00	0.00	0	20.0063432	-273300.000	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	
									8599.103

-3.192098970D+03 5.986807720D+01 3.055113902D+00 1.684673783D-03-3.287394830D-06  
3.095923617D-09-9.764691610D-13 -3.418443160D+04 3.294904120D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8599.103  
7.257089040D+05-1.484797741D+03 3.855527470D+00 7.138989850D-04-2.106757333D-07  
3.050092453D-11-1.639495583D-15 -2.355456660D+04-3.203856030D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8599.103  
1.764588423D+08-8.789998060D+04 1.886524859D+01-6.850866180D-04-1.403468022D-08  
1.503711045D-12-2.717518148D-17 6.853573220D+05-1.393231574D+02

HI                      Chase,1998 p1265.

2 j	9/61 H	1.00I	1.00	0.00	0.00	0.00	0	127.9124100	26359.000
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0

1.872881730D+04-3.431788840D+02 5.956712430D+00-8.543439600D-03 1.454780274D-05  
-1.049104164D-08 2.839734003D-12 3.682950720D+03-8.149756090D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8656.500  
4.724921450D+05-1.923465741D+03 5.758048970D+00-4.066266380D-04 9.474332050D-08  
-1.033534431D-11 4.611614790D-16 1.394857037D+04-1.182487652D+01

HNC                      Hf:Gurvich,1991 pt1 p227. Jacox,1998 p145.

2 g	6/01 H	1.00N	1.00C	1.00	0.00	0.00	0	27.0253400	194378.121
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
									10000.724

4.870620640D+04-9.891456250D+02 9.722153890D+00-1.113593916D-02 1.668862707D-05  
-1.113940941D-08 2.893600868D-12 2.664679758D+04-3.104826344D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10000.724  
1.198791660D+06-3.918941860D+03 9.118020090D+00-3.417761100D-04 3.314809680D-08  
-5.701574740D-13-7.789455390D-17 4.658810300D+04-3.468575882D+01

HNCO                      Hf:East,1993. Jacox,1998 p236.

2 g	7/00 H	1.00N	1.00C	1.000	1.00	0.00	0	43.0247400	-118056.529
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
									10966.126

7.542460080D+04-9.550937770D+02 6.725705870D+00 4.705687500D-03-4.959475510D-06  
3.694255120D-09-1.164859121D-12 -1.068149742D+04-1.365584762D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10966.126  
1.253216926D+06-5.021091540D+03 1.247789314D+01-6.891655250D-04 1.097738448D-07  
-9.306403800D-12 3.242606950D-16 1.453155559D+04-5.306419819D+01

HNO                      Gurvich,1989 pt1 p362 pt2 p227. Jacox,1998 p151.

2 g	10/01 H	1.00N	1.000	1.00	0.00	0.00	0	31.0140400	102032.725
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
									9941.880

-6.854764860D+04 9.551627200D+02-6.000720210D-01 7.995176750D-03-6.547079160D-07  
-3.670513400D-09 1.783392519D-12 6.435351260D+03 3.048166179D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9941.880  
-5.795614980D+06 1.945457427D+04-2.152568374D+01 1.797428992D-02-4.976040670D-06  
6.397924170D-10-3.142619368D-14 -1.104192372D+05 1.818650338D+02

HNO2                      Cis-trans. Gurvich,1989 pt1 p363 pt2 p228.

2 tpis89 H	1.00N	1.000	2.00	0.00	0.00	0	47.0134400	-78451.922	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	
									11597.285

8.591985060D+03 1.203644046D+02 9.412979120D-01 1.942891839D-02-2.253174194D-05  
1.384587594D-08-3.473550460D-12 -1.106337202D+04 2.073967331D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11597.285  
8.787904130D+05-3.990455030D+03 1.187349269D+01-4.881900610D-04 7.133636790D-08  
-5.376303340D-12 1.581778986D-16 1.246343241D+04-4.608874688D+01

HNO3                      Gurvich,1989 pt1 p367 pt2 p231.

2 g	5/99 H	1.00N	1.000	3.00	0.00	0.00	0	63.0128400	-133912.869
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
									11876.390

9.202869010D+03 1.093774496D+02-4.521042450D-01 2.984914503D-02-3.190635500D-05  
1.720931528D-08-3.782649830D-12 -1.764048507D+04 2.746644879D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11876.390  
-9.497809640D+04-2.733024468D+03 1.449426995D+01-7.821868050D-04 1.702693665D-07  
-1.930543961D-11 8.870455120D-16 -4.882517780D+03-5.928392985D+01

## Appendix D (continued)

HOCL Hf:Gurvich,1989 pt1 p187. Jacox,1998 p155.

2 g 1/01 H	1.000	1.00CL	1.00	0.00	0.00	0	52.4603400	-75740.032
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10224.626

-9.739307430D+03 3.547569520D+02 1.539514254D-01 1.617051795D-02-2.179693631D-05  
1.509103049D-08-4.125383510D-12 -1.176323791D+04 2.473257759D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10224.626  
8.530457810D+05-2.847760552D+03 7.948329040D+00-1.048782013D-04-1.482405043D-08  
4.591678270D-12-3.060073987D-16 7.250964950D+03-2.249831690D+01

HOF Gurvich,1989 pt1 p171 pt2 p79.

2 tps89 H	1.000	1.00F	1.00	0.00	0.00	0	36.0057432	-96898.221
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10088.435

-3.696888300D+04 7.809006660D+02-2.077685317D+00 2.038690173D-02-2.586919999D-05  
1.713797538D-08-4.551281870D-12 -1.631720064D+04 3.645052500D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10088.435  
8.812018230D+05-3.120013169D+03 8.223710070D+00-2.298036315D-04 1.459115709D-08  
1.095883303D-12-1.404445608D-16 6.300546710D+03-2.590150427D+01

HO2 Hf:Hills,1984 & NASA data. Jacox,1998 p153.

2 g 5/99 H	1.000	2.00	0.00	0.00	0.00	0	33.0067400	12020.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10002.162

-7.598882540D+04 1.329383918D+03-4.677388240D+00 2.508308202D-02-3.006551588D-05  
1.895600056D-08-4.828567390D-12 -5.873350960D+03 5.193602140D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10002.162  
-1.810669724D+06 4.963192030D+03-1.039498992D+00 4.560148530D-03-1.061859447D-06  
1.144567878D-10-4.763064160D-15 -3.200817190D+04 4.066850920D+01

HO2- B3LYP. EA: Oakes, 1985.

2 g 5/02 H	1.000	2.00E	1.00	0.00	0.00	0	33.0072886	-97923.080
298.150	1000.000	7	-2.0	-1.0	0.0	1.0	2.0	3.0
0.0								10245.320

1.103839835D+05-1.047963653D+03 6.360013990D+00 2.942520461D-03-6.284141340D-06  
5.438254240D-09-1.647305820D-12 0.000000000D+00-7.417741590D+03-1.251878002D+01  
1000.000 6000.000 7 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10245.320  
7.933306000D+05-2.503312417D+03 7.548962330D+00 8.308390150D-05-5.969730910D-08  
9.955377000D-12-5.606477280D-16 0.000000000D+00 2.512079084D+03-2.070065846D+01

HPO Hf:Gurvich,1989 pt1 p424. Jacox,1994 p46.

2 tps89 H	1.00P	1.000	1.00	0.00	0.00	0	47.9811010	-56868.759
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10065.343

-3.816314120D+04 7.927641870D+02-1.889940652D+00 1.800907425D-02-1.857631793D-05  
1.018768867D-08-2.355583619D-12 -1.157641240D+04 3.692925910D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10065.343  
3.842459450D+05-2.434951707D+03 8.582173920D+00-4.058448570D-04-1.669488740D-08  
2.253640566D-11-1.943063011D-15 5.761632120D+03-2.649097544D+01

HSO3F Chase,1998 p1057.

2 j 6/72 H	1.00S	1.000	3.00F	1.00	0.00	0	100.0695432	-753120.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15014.174

6.896242130D+03-9.305810750D+01 1.570331788D+00 3.780820750D-02-4.872720780D-05  
3.160796011D-08-8.189782930D-12 -9.180240820D+04 1.716315977D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15014.174  
5.544047080D+05-3.974424320D+03 1.778869264D+01-4.409322030D-04 5.944411390D-08  
-3.927015810D-12 8.891284000D-17 -7.153438270D+04-7.613127849D+01

H2 Ref-Elm. Gurvich,1978 pt1 p103 pt2 p31.

3 tps78 H	2.00	0.00	0.00	0.00	0.00	0	2.0158800	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8468.102

4.078323210D+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

H2+ Gurvich,1978 pt1 p107 pt2 p33.

3 tps78 H	2.00E	-1.00	0.00	0.00	0.00	0	2.0153314	1494672.430
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8583.103

-3.120886060D+04 2.304622909D+02 3.335564420D+00-2.419056763D-03 7.006022340D-06  
-5.610010660D-09 1.564169746D-12 1.774104638D+05-8.278523760D-01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8583.103  
1.672225964D+06-6.595184990D+03 1.279321925D+01-5.509345260D-03 2.030669412D-06  
-3.351027480D-10 1.946089104D-14 2.189999548D+05-6.792710780D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8583.103  
-1.822070983D+08 1.018196269D+05-1.245831898D+01 1.076647496D-03-3.932290360D-08  
6.285405030D-13-2.094721880D-18 -6.513101500D+05 1.471415370D+02

## Appendix D (continued)

H2- Chase,1998 p1312.

2 j 9/77 H	2.00E	1.00	0.00	0.00	0.00	0.00	0.00	2.0164286	235168.362
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.753565670D+04	1.221166236D+03	-2.264588838D+00	1.237202227D-02	-1.127100020D-05					
5.367239950D-09	-1.049420160D-12		2.121399948D+04	3.050556136D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.599275620D+04	-9.144682880D+02	5.149418810D+00	-1.016559478D-04	5.446919560D-08					
-6.155174450D-12	2.822451181D-16		3.234105180D+04	-1.440780980D+01					

HBOH Gurvich,1996a pt1 p44 pt2 p27.

2 g 9/98 H	2.00B	1.000	1.00	0.00	0.00	0.00	0.00	28.8262800	-48724.364
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.159644190D+04	1.223483035D+03	-5.460370510D+00	3.555388680D-02	-4.675020140D-05					
3.236008850D-08	-8.986053320D-12		-1.263659051D+04	5.422352290D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.534611049D+06	-5.753666430D+03	1.270893665D+01	-7.059628250D-04	1.027679375D-07					
-7.670926740D-12	2.211854768D-16		2.779370419D+04	-5.608860080D+01					

HCHO,formaldehy Hf:TRC(6/78) w-5300. Gurvich,1991 pt1 p62 pt2 p47.

2 g 5/01 H	2.00C	1.000	1.00	0.00	0.00	0.00	0.00	30.0259800	-108580.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.173916343D+05	1.873628846D+03	-6.890288570D+00	2.641561665D-02	-2.186389299D-05					
1.005693006D-08	-2.023476949D-12		-2.307351768D+04	6.420420550D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.700825405D+06	-7.620853840D+03	1.472447547D+01	-1.649111754D-03	3.292144720D-07					
-3.495049770D-11	1.526135000D-15		3.146812947D+04	-7.386478500D+01					

HCOOH Formic acid. Chao,1978.

2 g 6/01 H	2.00C	1.000	2.00	0.00	0.00	0.00	0.00	46.0253800	-378570.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.906279097D+04	7.658378880D+02	-3.328414130D+00	2.817542991D-02	-2.370050804D-05					
1.166063663D-08	-2.791373170D-12		-5.006443470D+04	4.387094230D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.872336450D+05	-7.632238080D+03	2.132788153D+01	-4.402546540D-03	1.102001695D-06					
-1.364343517D-10	6.648429750D-15		-5.781431910D+03	-1.111790688D+02					

H2F2 Gurvich,1989 vl pt1 p164 pt2 p308.

2 tpis89 H	2.00F	2.00	0.00	0.00	0.00	0.00	0.00	40.0126864	-569923.778
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.259214710D+04	-9.913544890D+02	1.043577115D+01	-2.407796033D-03	-6.376956160D-07					
2.735784900D-09	-1.104348590D-12		-6.572460830D+04	-3.038432132D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.464995601D+06	-3.335074920D+03	9.187487040D+00	1.051127249D-03	-3.278605570D-07					
4.456046230D-11	-2.281370136D-15		-4.825442090D+04	-2.639128168D+01					

H2O Hf:Cox,1989. Woolley,1987. TRC(10/88) tuv25.

2 g 8/89 H	2.000	1.00	0.00	0.00	0.00	0.00	0.00	18.0152800	-241826.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.947960830D+04	5.755731020D+02	9.317826530D-01	7.222712860D-03	-7.342557370D-06					
4.955043490D-09	-1.336933246D-12		-3.303974310D+04	1.724205775D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.034972096D+06	-2.412698562D+03	4.646110780D+00	2.291998307D-03	-6.836830480D-07					
9.426468930D-11	-4.822380530D-15		-1.384286509D+04	-7.978148510D+00					

H2O+ Gurvich,1989 pt1 p125 pt2 p38.

3 tpis89 H	2.000	1.00E	-1.00	0.00	0.00	0.00	0.00	18.0147314	981601.766
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.753892720D+03	2.249850054D+02	1.989400675D+00	6.117895160D-03	-7.095436640D-06					
5.547659470D-09	-1.704344789D-12		1.159585952D+05	1.135409642D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.228714260D+05	-2.864257487D+03	7.717565560D+00	-9.027801670D-04	6.177436860D-07					
-1.201457479D-10	7.407709940D-15		1.342086651D+05	-2.636617920D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.040922112D+07	-1.072691716D+03	1.131977392D+01	-7.364445000D-04	5.416450200D-08					
-1.900872342D-12	2.604761558D-17		1.042565942D+05	-5.467272320D+01					

H2O2 Hf:Gurvich,1989 pt1 p127. Gurvich,1978 pt1 p121.

2 g 6/99 H	2.000	2.00	0.00	0.00	0.00	0.00	0.00	34.0146800	-135880.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.279533580D+04	1.564748385D+03	-5.976460140D+00	3.270744520D-02	-3.932193260D-05					
2.509255235D-08	-6.465045290D-12		-2.494004728D+04	5.877174180D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.489428027D+06	-5.170821780D+03	1.128204970D+01	-8.042397790D-05	-1.818383769D-08					
6.947265590D-12	-4.827831900D-16		1.418251038D+04	-4.650855660D+01					

## Appendix D (continued)

H2S Gurvich,1989 pt1 p298 pt2 p181.

2 g 4/01 H	2.00S	1.00	0.00	0.00	0.00	0.00	0	34.0808800	-20600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.543808810D+03	-6.875175080D+01	4.054921960D+00	-3.014557336D-04	3.768497750D-06					
-2.239358925D-09	3.086859108D-13		-3.278457280D+03	1.415194691D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.430040220D+06	-5.284028650D+03	1.016182124D+01	-9.703849960D-04	2.154003405D-07					
-2.169695700D-11	9.318163070D-16		2.908696214D+04	-4.349160391D+01					

H2SO4 Gurvich,1989 pt1 p300 pt2 p182.

2 tps89 H	2.00S	1.000	4.00	0.00	0.00	0	98.0784800	-732731.721	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.129150050D+04	6.681589890D+02	-2.632753507D+00	5.415382480D-02	-7.067502230D-05					
4.684611420D-08	-1.236791238D-11		-9.315660120D+04	3.961096201D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.437877914D+06	-6.614902530D+03	2.157662058D+01	-4.806255970D-04	3.010775121D-08					
2.334842469D-12	-2.946330375D-16		-5.259092950D+04	-1.023603724D+02					

H2BOH Gurvich,1996a pt1 p46 pt2 p29.

2 tps96 H	3.00B	1.000	1.00	0.00	0.00	0	29.8342200	-289633.898	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.686766780D+04	1.820335089D+03	-1.032373881D+01	4.922801060D-02	-5.978619910D-05					
3.946062730D-08	-1.068442257D-11		-4.415238150D+04	7.986177290D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.294795193D+06	-9.382923560D+03	1.798228329D+01	-1.506116214D-03	2.635641095D-07					
-2.483163637D-11	9.736759120D-16		2.039738953D+04	-9.448201210D+01					

HB(OH)2 Gurvich,1996a pt1 p47 pt2 p30.

2 tps96 H	3.00B	1.000	2.00	0.00	0.00	0	45.8336200	-644438.724	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.067044022D+04	9.534459160D+02	-8.088956520D+00	5.972425290D-02	-8.071336320D-05					
5.612118350D-08	-1.553607566D-11		-8.264270810D+04	6.539571640D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.122674609D+06	-8.615948940D+03	1.966179520D+01	-8.148411500D-04	8.955082040D-08					
-3.344830510D-12	-6.919578140D-17		-2.788790377D+04	-9.983559610D+01					

H3BO3 Gurvich,1996a pt1 p50 pt2 p32.

2 tps96 H	3.00B	1.000	3.00	0.00	0.00	0	61.8330200	-1004360.442	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.568901843D+04	1.138029495D+02	-4.045096580D+00	5.924521680D-02	-8.148028410D-05					
5.658593290D-08	-1.549277050D-11		-1.221702050D+05	4.132220140D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.297369132D+06	-8.933571790D+03	2.193496552D+01	-3.094783490D-04	-5.064052990D-08					
1.482296684D-11	-9.764420900D-16		-6.970298470D+04	-1.122292829D+02					

H3B3O3 Gurvich,1996a pt1 p53 pt2 p34.

2 tps96 H	3.00B	3.000	3.00	0.00	0.00	0	83.4550200	-1203760.987	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.985284188D+05	4.104132090D+03	-2.827215617D+01	1.269639253D-01	-1.558505781D-04					
9.966304070D-08	-2.603677650D-11		-1.648494375D+05	1.763917407D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.286220713D+06	-1.093258784D+04	3.213518670D+01	-2.595402269D-03	5.353766470D-07					
-5.833567380D-11	2.600757913D-15		-8.752856890D+04	-1.770847815D+02					

H3B3O6 Gurvich,1996a pt1 p55 pt2 p35.

2 tps96 H	3.00B	3.000	6.00	0.00	0.00	0	131.4532200	-2263687.611	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.067031503D+04	7.083391540D+02	-7.123820950D+00	1.025049979D-01	-1.295004602D-04					
8.322737590D-08	-2.145746724D-11		-2.778049216D+05	6.063597630D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.952433352D+06	-1.154932896D+04	3.892676110D+01	-1.113852280D-03	1.280317726D-07					
-5.728464820D-12	-2.214529572D-17		-2.120927136D+05	-2.075566801D+02					

H3F3 Gurvich,1989 pt1 p166 pt2 p309.

2 tps89 H	3.00F	3.00	0.00	0.00	0.00	0	60.0190296	-883676.790	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.888562650D+04	-1.380212880D+03	8.980458470D+00	1.871609057D-02	-3.127862508D-05					
2.589436165D-08	-8.040372270D-12		-1.013661491D+05	-2.585302557D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.515790373D+06	-8.789423320D+03	2.023933445D+01	-1.131704646D-03	1.692779921D-07					
-1.308662105D-11	3.978322000D-16		-5.471713650D+04	-9.907787640D+01					

## Appendix D (continued)

H3O+ Gurvich,1989 pt1 p130 pt2 p41.

3 tps89 H	3.000	1.00E	-1.00	0.00	0.00	0	19.0226714	598000.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-6.447640150D+04	1.181817922D+03	-3.801893060D+00	2.220628313D-02	-2.445343237D-05				
1.573297747D-08	-4.158836410D-12		6.530613320D+04	4.282723130D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
2.955126200D+06	-9.185669410D+03	1.341398696D+01	-5.590339210D-04	1.138387119D-08				
7.259927210D-12	-6.133734360D-16		1.290534257D+05	-7.021828180D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-1.591228592D+07	4.898727210D+03	8.881336820D+00	1.299244015D-04	-8.169245590D-09				
2.649115685D-13	-3.472865280D-18		2.090178405D+04	-3.217683350D+01				

(HCOOH)2 Formic acid dimer. Chao,1978.

2 g 6/01 H	4.00C	2.000	4.00	0.00	0.00	0	92.0507600	-820942.640
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-2.001447991D+05	3.502457370D+03	-1.853488051D+01	9.547467130D-02	-1.059184484D-04				
6.323086900D-08	-1.567561216D-11		-1.172621688D+05	1.319646887D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
3.308188420D+06	-1.633668256D+04	3.751348820D+01	-3.148108995D-03	6.008707760D-07				
-6.144462500D-11	2.600562474D-15		-6.265894440D+03	-2.107476941D+02				

H4F4 Gurvich,1989 pt1 p167 pt2 p310.

2 tps89 H	4.00F	4.00	0.00	0.00	0.00	0	80.0253728	-1186932.336
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
1.315109024D+05	-1.840361560D+03	1.264093152D+01	2.495407360D-02	-4.170394610D-05				
3.452523840D-08	-1.072034360D-11		-1.364003454D+05	-4.122913530D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
3.354037990D+06	-1.171922040D+04	2.765243565D+01	-1.508934621D-03	2.257027572D-07				
-1.744867255D-11	5.304351740D-16		-7.420213160D+04	-1.388603332D+02				

H5F5 Gurvich,1989 pt1 p168 pt2 p311.

2 tps89 H	5.00F	5.00	0.00	0.00	0.00	0	100.0317160	-1490187.882
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
1.641361897D+05	-2.300510396D+03	1.630140545D+01	3.119205422D-02	-5.212926350D-05				
4.315611240D-08	-1.340031413D-11		-1.714345408D+05	-5.682157380D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
4.192290730D+06	-1.464903043D+04	3.506554920D+01	-1.886170471D-03	2.821289954D-07				
-2.181090984D-11	6.630474160D-16		-9.368704200D+04	-1.788592044D+02				

H6F6 Gurvich,1989 pt1 p169 pt2 p312.

2 tps89 H	6.00F	6.00	0.00	0.00	0.00	0	120.0380592	-1805545.131
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
1.956886618D+05	-2.753909880D+03	1.975625055D+01	3.807717010D-02	-6.341218880D-05				
5.219233290D-08	-1.612185649D-11		-2.079269410D+05	-7.113607980D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
5.024520320D+06	-1.742817868D+04	4.214870500D+01	-2.084564791D-03	2.930051519D-07				
-2.052079159D-11	5.206937300D-16		-1.154497653D+05	-2.163947001D+02				

H7F7 Gurvich,1989 pt1 p170 pt2 p313.

2 tps89 H	7.00F	7.00	0.00	0.00	0.00	0	140.0444024	-2099698.974
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
2.293867477D+05	-3.220807860D+03	2.362235212D+01	4.366801880D-02	-7.297990340D-05				
6.041786420D-08	-1.876025627D-11		-2.418637479D+05	-8.838812260D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
5.868789830D+06	-2.050863473D+04	4.989176110D+01	-2.640634895D-03	3.949796330D-07				
-3.053515088D-11	9.282601780D-16		-1.330177809D+05	-2.592385142D+02				

He Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.

3 g 5/97 HE	1.00	0.00	0.00	0.00	0.00	0	4.0026020	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
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								
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								
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				

## Appendix D (continued)

He+ Moore,1971; Moore,1970a. Gordon,1999.

3 g 3/97 HE	1.00E	-1.00	0.00	0.00	0.00	0.00	0	4.0020534	2378521.473
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							2.853233739D+05	1.621665557D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							2.853233739D+05	1.621665557D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							2.853233739D+05	1.621665557D+00

Hg Hf:Cox,1989. Moore,1971. Gordon,1999.

3 g 1/98 HG	1.00	0.00	0.00	0.00	0.00	0	200.5900000	61380.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							6.636900080D+03	6.800201540D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.146573510D+04	-1.681269855D+02	2.718343098D+00	-1.445026192D-04	5.158977660D-08					
-9.472485010D-12	7.034797406D-16							7.688684930D+03	5.271236090D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.358443930D+08	-4.433853810D+05	1.463223992D+02	-2.318441669D-02	1.916335174D-06					
-7.419662000D-11	1.067224054D-15							3.391999920D+06	-1.201225990D+03

Hg+ Moore,1971. Gordon,1999.

3 g 7/97 HG	1.00E	-1.00	0.00	0.00	0.00	0	200.5894514	1074643.128	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.098344940D-04	-4.343581620D-06	2.500000019D+00	-4.389036810D-11	5.563969200D-14					
-3.638228260D-17	9.607881995D-21							1.285037483D+05	7.493344500D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.229984728D+04	2.732269908D+01	2.484182160D+00	-4.426797610D-06	7.489685860D-09					
-2.549887287D-12	2.819873366D-16							1.283188257D+05	7.625244570D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.498617710D+07	3.775543500D+04	-7.155545550D+00	1.170310234D-03	-7.931471440D-08					
4.029174000D-12	-7.741071633D-17							-1.676894201D+05	9.116750020D+01

HgBr2 Hf: Pankratz,1984. Chase,1998 p485 3/62.

2 g12/00 HG	1.00BR	2.00	0.00	0.00	0.00	0	360.3980000	-91311.616	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.991826537D+03	-1.902186083D+02	8.246401260D+00	-1.607089392D-03	1.947654549D-06					
-1.242873546D-09	3.241818310D-13							-1.230723096D+04	-8.716659300D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.243649290D+04	-3.312652270D+00	7.502765170D+00	-1.202360213D-06	2.830526999D-10					
-3.407686700D-14	1.640497921D-18							-1.327483366D+04	-4.368555600D+00

I Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.

3 g 3/97 I	1.00	0.00	0.00	0.00	0.00	0	126.9044700	106760.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.698199675D+02	-2.716437233D+00	2.517385557D+00	-5.730692070D-05	1.031716184D-07					
-9.670641930D-11	3.706471651D-14							1.210750090D+04	7.405823130D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.785860570D+05	2.303279568D+03	2.886686091D-03	1.180878463D-03	-2.264074866D-07					
1.963511339D-11	-6.243525941D-16							-2.616792742D+03	2.558922997D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.747630780D+07	-8.681111190D+04	3.950617020D+01	-6.514063250D-03	5.380695340D-07					
-1.969145066D-11	2.643177163D-16							6.384843030D+05	-2.972997119D+02

I+ Moore,1971. Moore,1970a. Gordon,1999.

3 g10/97 I	1.00E	-1.00	0.00	0.00	0.00	0	126.9039214	1121351.028	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.014969010D+02	8.139052610D+00	2.470174760D+00	4.161393820D-05	7.133397860D-09					
-7.105950140D-11	4.873766102D-14							1.340794213D+05	7.903420090D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.788385330D+05	2.404962651D+03	-1.791751142D-01	1.227311979D-03	-1.801494030D-07					
9.923983960D-12	-9.775286439D-17							1.188531631D+05	2.710544347D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.314420010D+08	3.971131910D+05	-9.860191990D+01	1.358236563D-02	-9.920747650D-07					
3.684927700D-11	-5.301687095D-16							-3.001474591D+06	8.790468740D+02

## Appendix D (continued)

I- Hotop,1985. Gordon,1999.

3 g10/97 I	1.00E	1.00	0.00	0.00	0.00	0	126.9050186	-194595.572
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00						-2.414970936D+04	6.113465380D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00						-2.414970936D+04	6.113465380D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00						-2.414970936D+04	6.113465380D+00

IF5 Gurvich,1989 pt1 p232 pt2 p123.

2 tpis89 I	1.00F	5.00	0.00	0.00	0.00	0	221.8964860	-841000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.026184530D+05	-3.598183170D+03	2.530349738D+01	-1.348602458D-02	1.105687229D-05				
-4.707939510D-09	7.864411470D-13						-8.700147250D+04	-1.112719941D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.620506260D+05	-1.639236093D+02	1.612272743D+01	-4.914431550D-05	1.086015052D-08				
-1.244672691D-12	5.763593620D-17						-1.061642293D+05	-5.398773360D+01

IF7 Gurvich,1989 pt1 p234 pt2 p124.

2 tpis89 I	1.00F	7.00	0.00	0.00	0.00	0	259.8932924	-961500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.999853564D+05	-5.501554130D+03	3.627133980D+01	-2.095765818D-02	1.761972680D-05				
-7.829142330D-08	1.405939372D-12						-9.331307660D+04	-1.754216150D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.614422640D+05	-2.646288326D+02	2.219879891D+01	-7.984221470D-05	1.768835964D-08				
-2.031523755D-12	9.423767390D-17						-1.225245322D+05	-8.774010730D+01

I2 Gurvich,1989 pt1 p220 pt2 p117.

2 tpis89 I	2.00	0.00	0.00	0.00	0.00	0	253.8089400	62420.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.087968770D+03	-1.249585210D+01	4.504219090D+00	1.370962533D-04	-1.390523014D-07				
1.174813853D-10	2.337541043D-14						6.213469810D+03	5.583836940D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.632594160D+06	1.793961560D+04	-1.723055169D+01	1.244214080D-02	-3.332768580D-06				
4.125477940D-10	-1.960461713D-14						-1.068505292D+05	1.600531883D+02

In Hf:Gurvich,1996a. Johansson,1966. Moore,1971. Gordon,1999.

3 g 1/99 IN	1.00	0.00	0.00	0.00	0.00	0	114.8180000	240700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.149518050D+04	-9.177999020D+02	8.938687950D+00	-2.224112602D-02	3.823881940D-05				
-2.890116948D-08	8.047481221D-12						3.239031620D+04	-2.764567028D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.683608899D+06	2.210473186D+03	3.472219370D+00	-1.082267422D-03	3.479699980D-07				
-5.158092410D-11	3.183043089D-15						1.095965206D+04	2.557189088D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.289146601D+06	3.908691060D+04	-1.789204885D+01	3.655375250D-03	-2.576493626D-07				
7.929188320D-12	-9.066642170D-17						-2.376257502D+05	1.738048645D+02

In+ IP:Johansson,1966. Moore,1971. Gordon,1999.

3 g 4/99 IN	1.00E	-1.00	0.00	0.00	0.00	0	114.8174514	6996.425
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.150488908D-01	-2.523854672D-03	2.500011877D+00	-2.869063919D-08	3.753870400D-11				
-2.525942419D-14	6.842932660D-18						9.610930170D+01	5.963254400D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.536995140D+04	-1.445142103D+02	2.681812441D+00	-1.157480060D-04	3.947714810D-08				
-6.879243620D-12	4.819204920D-16						1.004261440D+03	4.683759180D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.188028020D+07	1.322640301D+04	7.453303840D+00	-1.893250634D-03	2.114636410D-07				
-8.432019810D-12	1.185570972D-16						-1.335858982D+05	-2.765870435D+01

InBr Gurvich,1996a pt1 p291 pt2 p233

2 tpis96 IN	1.00BR	1.00	0.00	0.00	0.00	0	194.7220000	-54115.879
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.540851435D+03	-5.294704710D+01	4.717438090D+00	-4.344669490D-04	6.513513640D-07				
-4.403995150D-10	1.234046209D-13						-7.607594280D+03	4.258881000D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.948374420D+05	-2.318183711D+03	7.032889580D+00	-1.245920568D-03	3.276693350D-07				
-3.003771106D-11	5.853192770D-16						6.957627290D+03	-1.273502660D+01

## Appendix D (continued)

InBr2                    Gurvich,1996a pt1 p292 pt2 p234.

2 tpis96 IN	1.00BR	2.00	0.00	0.00	0.00	0	274.6260000	-149729.059
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.619878900D+01	-2.365897310D+02	7.926545160D+00	-1.994547959D-03	2.420414153D-06				
-1.548924922D-09	4.058148390D-13		-1.895355588D+04	-5.338867540D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.217162030D+05	4.792682100D+02	7.102649480D+00	-5.514019780D-04	3.157862421D-07				
-5.511254510D-11	3.172161390D-15		-2.370923659D+04	1.193263347D-01				

InBr3                    Gurvich,1996a pt1 p292 pt2 p236.

2 tpis96 IN	1.00BR	3.00	0.00	0.00	0.00	0	354.5300000	-256587.267
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.990115300D+03	-2.805930452D+02	1.110356060D+01	-2.379995808D-03	2.887825281D-06				
-1.844500707D-09	4.814395870D-13		-3.250504910D+04	-1.871748987D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.505783100D+04	-4.858721320D+00	1.000406131D+01	-1.767620958D-06	4.164016060D-10				
-5.015528870D-14	2.415414123D-18		-3.393179240D+04	-1.229069868D+01				

InCL                    Gurvich,1996a pt1 p281 pt2 p225

2 tpis96 IN	1.00CL	1.00	0.00	0.00	0.00	0	150.2710000	-72147.883
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.430713030D+03	-2.178267726D+02	5.418830900D+00	-2.048005100D-03	2.702295936D-06				
-1.795319798D-09	4.847469090D-13		-8.959841070D+03	-1.202999253D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.745751636D+05	8.940986910D+02	3.268118390D+00	9.180277780D-04	-3.083262431D-07				
5.745458810D-11	3.645275750D-15		-1.561603430D+04	1.266880374D+01				

InCL2                    Gurvich,1996a pt1 p283 pt2 p226.

2 tpis96 IN	1.00CL	2.00	0.00	0.00	0.00	0	185.7240000	-201483.416
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.935164870D+03	-4.172101860D+02	8.588494910D+00	-3.348385610D-03	3.997866640D-06				
-2.525301853D-09	6.544490330D-13		-2.426480269D+04	-1.164521725D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.328719840D+05	4.757691610D+02	7.105443690D+00	-5.525786960D-04	3.160567738D-07				
-5.514453680D-11	3.173680380D-15		-2.995095917D+04	-2.294555511D+00				

InCL3                    Gurvich,1996a pt1 p286 pt2 p228.

2 tpis96 IN	1.00CL	3.00	0.00	0.00	0.00	0	221.1770000	-369693.227
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.614743044D+04	-8.414604560D+02	1.311784790D+01	-6.435282470D-03	7.554874750D-06				
-4.705078560D-09	1.204213663D-12		-4.326469580D+04	-3.500080940D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.114043630D+04	-1.628425068D+01	1.001309622D+01	-5.544528880D-06	1.279877732D-09				
-1.518261505D-13	7.226562770D-18		-4.758974170D+04	-1.669761011D+01				

InF                    Gurvich,1996a pt1 p272 pt2 p217.

2 tpis96 IN	1.00F	1.00	0.00	0.00	0.00	0	133.8164032	-193419.989
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.190123320D+04	-5.295254260D+02	6.172886260D+00	-2.986035832D-03	3.233778030D-06				
-1.856975575D-09	4.465024970D-13		-2.187176282D+04	-7.591216620D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.689001200D+05	1.321019051D+03	2.881329353D+00	1.041591078D-03	-3.090754867D-07				
4.926646560D-11	-2.699156425D-15		-3.308369810D+04	1.396688303D+01				

InF2                    Gurvich,1996a pt1 p274 pt2 p218.

2 tpis96 IN	1.00F	2.00	0.00	0.00	0.00	0	152.8148064	-457186.824
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.522480210D+04	-1.088616881D+03	9.481705210D+00	-2.893229367D-03	1.516224649D-06				
-7.989517810D-11	-1.466781026D-13		-5.124336150D+04	-2.146666090D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.318960340D+05	-1.688472420D+03	8.925863010D+00	-1.049188835D-03	2.723934190D-07				
-2.882959902D-11	1.073493779D-15		-4.673691940D+04	-1.932464363D+01				

InF3                    Gurvich,1996a pt1 p276 pt2 p220.

2 tpis96 IN	1.00F	3.00	0.00	0.00	0.00	0	171.8132096	-863079.566
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.071608336D+05	-1.660071901D+03	1.395972813D+01	-5.018693260D-03	3.226367530D-06				
-7.823385970D-10	-3.726999800D-14		-9.795214990D+04	-4.606353470D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.656855506D+05	-7.965889290D+01	1.005913347D+01	-2.350816639D-05	5.163512930D-09				
-5.888048810D-13	2.715090697D-17		-1.068682627D+05	-2.132968218D+01				



## Appendix D (continued)

InH Gurvich,1996a pt1 p269 pt2 p215  
 2 tps96 IN 1.00H 1.00 0.00 0.00 0.00 0 115.8259400 215016.904  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8684.104  
 -5.152828720D+04 7.813792590D+02-8.433385340D-01 1.044471274D-02-9.761074820D-06  
 4.540635200D-09-8.169906900D-13 2.110048908D+04 2.939346222D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8684.104  
 7.797406660D+05-3.646882080D+03 9.542967350D+00-3.481281720D-03 1.304805603D-06  
 -2.182950701D-10 1.274009748D-14 4.643295460D+04-3.659329230D+01

InI Gurvich,1996a pt1 p298 pt2 p241.  
 2 tps96 IN 1.00I 1.00 0.00 0.00 0.00 0 241.7224700 26417.124  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10271.124  
 -4.686348740D+02-5.685530990D+01 4.781849690D+00-6.619368310D-04 1.027666742D-06  
 -7.270592070D-10 2.077991102D-13 2.095570254D+03 4.885515130D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10271.124  
 1.529221772D+06-4.690373680D+03 1.004593462D+01-3.140434110D-03 9.460834390D-07  
 -1.253862848D-10 5.949805640D-15 3.152478143D+04-3.297697490D+01

InI2 Gurvich,1996a pt1 p300 pt2 p243.  
 2 tps96 IN 1.00I 2.00 0.00 0.00 0.00 0 368.6269400 -39460.643  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14912.757  
 -4.513890600D+03-1.183726870D+02 7.473110080D+00-1.034474090D-03 1.271465534D-06  
 -8.227820300D-10 2.178307019D-13 -6.278536040D+03-6.667297500D-01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14912.757  
 -3.130671665D+05 4.813810700D+02 7.100914180D+00-5.506559920D-04 3.156120735D-07  
 -5.509170540D-11 3.171162830D-15 -1.043012750D+04 2.141662307D+00

InI3 Gurvich,1996a pt1 p301 pt2 p245.  
 2 tps96 IN 1.00I 3.00 0.00 0.00 0.00 0 495.5314100 -105435.914  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20852.086  
 -8.782397170D+03-1.265914859D+02 1.050659120D+01-1.106109314D-03 1.354335766D-06  
 -8.709453460D-10 2.285186350D-13 -1.508269063D+04-1.211411745D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20852.086  
 -2.196742567D+04-2.151167521D+00 1.000182200D+01-8.002214700D-07 1.897343164D-10  
 -2.296252460D-14 1.109838196D-18 -1.572406335D+04-9.170888690D+00

InO Gurvich,1996a pt1 p261 pt2 p212  
 2 tps96 IN 1.00O 1.00 0.00 0.00 0.00 0 130.8174000 145993.109  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9042.109  
 -1.154727169D+05 1.753668703D+03-6.965033810D+00 2.961698958D-02-3.123332334D-05  
 1.437244720D-08-2.235519898D-12 8.188679590D+03 6.608621260D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9042.109  
 -8.052130950D+05 1.693064203D+03 4.760863580D+00-7.340718400D-04 3.229597760D-07  
 -4.580150380D-11 1.954611725D-15 4.005519810D+03 3.500742460D+00

InOH Gurvich,1996a pt1 p271 pt2 p216.  
 2 tps96 IN 1.00O 1.00H 1.00 0.00 0.00 0 131.8253400 -124447.344  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10736.839  
 6.123463020D+04-1.195863129D+03 1.041427981D+01-6.870002500D-03 6.214128780D-06  
 -2.408203181D-09 3.177641780D-13 -1.079852170D+04-3.189890840D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10736.839  
 8.525128930D+05-2.350317172D+03 7.984515140D+00 9.915815620D-05-6.212385450D-08  
 1.016169575D-11-5.682557640D-16 -1.536213610D+03-2.043107643D+01

In2Br2 Gurvich,1996a pt1 p294 pt2 p237.  
 2 tps96 IN 2.00BR 2.00 0.00 0.00 0.00 0 389.4440000 -196305.215  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21434.943  
 -9.221188300D+03-3.616677030D+01 1.014728771D+01-3.255775200D-04 4.022327480D-07  
 -2.604080237D-10 6.867689550D-14 -2.644883479D+04-1.000360073D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21434.943  
 -1.290781804D+04-6.075401240D-01 1.000052163D+01-2.312058331D-07 5.517315720D-11  
 -6.708620190D-15 3.253841650D-19 -2.663136878D+04-9.149949470D+00

In2Br4 Gurvich,1996a pt1 p295 pt2 p238.  
 2 tps96 IN 2.00BR 4.00 0.00 0.00 0.00 0 549.2520000 -436508.683  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31798.117  
 -1.425555379D+04-2.866009341D+02 1.713866292D+01-2.473506655D-03 3.017273071D-06  
 -1.934900430D-09 5.065874250D-13 -5.593753060D+04-3.837105980D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31798.117  
 -4.453463710D+04-4.911523980D+00 1.600413764D+01-1.810579975D-06 4.281715740D-10  
 -5.171998020D-14 2.496142837D-18 -5.739175410D+04-3.174906390D+01

## Appendix D (continued)

In2Br6                      Gurvich,1996a pt1 p296 pt2 p239.

2	tpis96	IN	2.00BR	6.00	0.00	0.00	0.00	0.00	0	709.0600000	-628683.430
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											43096.728

-1.758940752D+04-4.859034480D+02 2.391654505D+01-4.142061490D-03 5.033849320D-06  
-3.219103650D-09 8.410220070D-13                      -7.988844460D+04-6.437871880D+01  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      43096.728  
-6.945039480D+04-8.402368170D+00 2.200703884D+01-3.068251799D-06 7.235965730D-10  
-8.722870580D-14 4.203469910D-18                      -8.235759850D+04-5.322192800D+01

In2CL2                      Gurvich,1996a pt1 p287 pt2 p229.

2	tpis96	IN	2.00CL	2.00	0.00	0.00	0.00	0	300.5420000	-232177.375	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											20223.895

-1.142848747D+04-1.416015827D+02 1.056853314D+01-1.244253440D-03 1.526076784D-06  
-9.826402810D-10 2.580766990D-13                      -3.026327087D+04-1.565104960D+01  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      20223.895  
-2.616606332D+04-2.401955489D+00 1.000203984D+01-8.975190030D-07 2.130755553D-10  
-2.581140900D-14 7.245404540D-18                      -3.098016735D+04-1.234946505D+01

In2CL4                      Gurvich,1996a pt1 p287 pt2 p230.

2	tpis96	IN	2.00CL	4.00	0.00	0.00	0.00	0	371.4480000	-579125.856	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											29456.525

9.814083080D+03-8.488959010D+02 1.923410360D+01-6.815674240D-03 8.129220730D-06  
-5.125076850D-09 1.324324755D-12                      -7.027688140D+04-5.582665695D+01  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      29456.525  
-8.503771790D+04-1.552464614D+01 1.601269668D+01-5.441549870D-06 1.267594997D-09  
-1.514110365D-13 7.245404540D-18                      -7.461921740D+04-3.691150615D+01

In2CL6                      Gurvich,1996a pt1 p288 pt2 p231.

2	tpis96	IN	2.00CL	6.00	0.00	0.00	0.00	0	442.3540000	-882340.029	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											38423.462

3.004663159D+04-1.585621359D+03 2.796489470D+01-1.245506052D-02 1.475341213D-05  
-9.252689200D-09 2.381233885D-12                      -1.048828300D+05-9.788404640D+01  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      38423.462  
-1.499400484D+05-2.988680816D+01 2.202425362D+01-1.033652301D-05 2.397911922D-09  
-2.855307516D-13 1.363051661D-17                      -1.130110233D+05-6.293985680D+01

In2F2                      Gurvich,1996a pt1 p276 pt2 p221.

2	tpis96	IN	2.00F	2.00	0.00	0.00	0.00	0	267.6328064	-532234.300	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											18039.900

7.255717100D+03-6.448265650D+02 1.247539512D+01-5.246089620D-03 6.283616210D-06  
-3.974342340D-09 1.029559356D-12                      -6.384892450D+04-3.108004586D+01  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      18039.900  
-6.409715440D+04-1.163740672D+01 1.000956511D+01-4.114086910D-06 9.608828320D-10  
-1.150013486D-13 5.511437480D-18                      -6.714277850D+04-1.661718474D+01

In2F4                      Gurvich,1996a pt1 p277 pt2 p222.

2	tpis96	IN	2.00F	4.00	0.00	0.00	0.00	0	305.6296128	-1284788.126	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											24763.074

1.225213611D+05-2.444998374D+03 2.342425457D+01-1.291427120D-02 1.308700476D-05  
-7.181673930D-09 1.648386404D-12                      -1.466942111D+05-8.943560050D+01  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      24763.074  
-2.205977486D+05-7.822083770D+01 1.605923872D+01-2.394023240D-05 5.329582790D-09  
-6.144609570D-13 2.859099598D-17                      -1.595716347D+05-4.469574580D+01

In2F6                      Gurvich,1996a pt1 p279 pt2 p223.

2	tpis96	IN	2.00F	6.00	0.00	0.00	0.00	0	343.6264192	-1960000.000	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											33567.102

1.825490583D+05-3.552111710D+03 3.275425230D+01-1.868064635D-02 1.892443162D-05  
-1.038916311D-08 2.386637271D-12                      -2.239648760D+05-1.363626758D+02  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      33567.102  
-3.170966380D+05-1.167440973D+02 2.208847456D+01-3.577733930D-05 7.968959040D-09  
-9.191681700D-13 4.278494150D-17                      -2.426661118D+05-7.155328560D+01

In2I2                      Gurvich,1996a pt1 p303 pt2 p246.

2	tpis96	IN	2.00I	2.00	0.00	0.00	0.00	0	483.4449400	-27813.524	
			200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
											22058.476

-6.681925010D+03-1.449103222D+01 1.005929122D+01-1.314921486D-04 1.628373589D-07  
-1.056087811D-10 2.788963879D-14                      -6.279602600D+03-7.291130980D+00  
1000.000      6000.0007   -2.0   -1.0   0.0   1.0   2.0   3.0   4.0   0.0                      22058.476  
-8.148157300D+03-2.444544443D-01 1.000021086D+01-9.376789250D-08 2.242988180D-11  
-2.732299303D-15 1.327135699D-19                      -6.352651500D+03-6.947725420D+00

## Appendix D (continued)

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In2I4          Gurvich,1996a pt1 p304 pt2 p247.
  2 tpis96 IN  2.00I  4.00  0.00  0.00  0.00  0  737.2538800  -199143.181
    200.000  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      33468.979
-1.501028064D+04-9.744797900D+01 1.639383950D+01-8.659380210D-04 1.065671801D-06
-6.879252680D-10 1.810240886D-13      -2.830388443D+04-2.986294828D+01
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      33468.979
-2.505699251D+04-1.642155234D+00 1.600140149D+01-6.187066280D-07 1.472308565D-10
-1.786593333D-14 8.652338780D-19      -2.879655333D+04-2.757790375D+01
In2I6          Gurvich,1996a pt1 p305 pt2 p248.
  2 tpis96 IN  2.00I  6.00  0.00  0.00  0.00  0  991.0628200  -319720.040
    200.000  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      45088.120
-2.232640607D+04-2.000786874D+02 2.280417927D+01-1.761331313D-03 2.161510393D-06
-1.392400447D-09 3.658171880D-13      -4.412547680D+04-5.273802030D+01
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      45088.120
-4.311905850D+04-3.390350590D+00 2.200288128D+01-1.268348706D-06 3.012121900D-10
-3.649676710D-13 1.765530622D-18      -4.513820270D+04-4.806868370D+01
In2O          Gurvich,1996a pt1 p264 pt2 p213.
  2 tpis96 IN  2.00O  1.00  0.00  0.00  0.00  0  245.6354000  -34763.707
    200.000  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12796.504
  5.065653500D+04-8.070363670D+02 8.642067270D+00-1.533035446D-03 2.866419382D-07
  4.981134970D-10-2.554320291D-13      -1.924908459D+03-1.490718759D+01
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12796.504
-9.232786360D+04-5.201127280D+01 7.038723620D+00-1.543821179D-05 3.399700870D-09
-3.885457100D-13 1.795125270D-17      -6.270926800D+03-4.421820410D+00
K          Hf:Cox,1989. Sugar,1985. Gordon 1999.
  3 g 7/97 K  1.00  0.00  0.00  0.00  0.00  0  39.0983000  89000.000
    200.000  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  9.665143930D+00-1.458059455D-01 2.500865861D+00-2.601219276D-06 4.187306580D-09
-3.439722110D-12 1.131569009D-15      9.959493490D+03 5.035822260D+00
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
-3.566422360D+06 1.085289825D+04-1.054134898D+01 8.009801350D-03-2.696681041D-06
  4.715294150D-10-2.976897350D-14      -5.875337010D+04 9.738551240D+01
    6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  9.205786590D+08-6.935300280D+05 1.911270788D+02-2.305931672D-02 1.430294866D-06
-4.409335020D-11 5.366769166D-16      5.395082190D+06-1.622158805D+03
K+          Sugar,1985. Gordon 1999.
  3 g 6/97 K  1.00E -1.00  0.00  0.00  0.00  0  39.0977514  514007.528
    298.150  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00      6.107516860D+04 4.347404440D+00
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00      6.107516860D+04 4.347404440D+00
    6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  2.177901245D+07-1.415076630D+04 6.248954270D+00-5.187436800D-04 3.959640680D-08
-1.584335542D-12 2.603558905D-17      1.722753576D+05-2.781728990D+01
K-          Hotop,1985. Gordon 1999.
  3 g 9/97 K  1.00E  1.00  0.00  0.00  0.00  0  39.0988486  34418.128
    298.150  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00      3.394150710D+03 4.347446530D+00
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00      3.394150710D+03 4.347446530D+00
    6000.000  20000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      6197.428
  0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00      3.394150710D+03 4.347446530D+00
KALF4          Gurvich,1982 pt1 p417 pt2 p441.
  2 tpis82 K  1.00AL  1.00F  4.00  0.00  0.00  0  142.0734508  -1907856.822
    200.000  1000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      21421.391
  1.199327246D+05-2.156457352D+03 1.815348004D+01 3.115762809D-03-9.511991670D-06
  8.431756230D-09-2.615583061D-12      -2.222545809D+05-6.823299970D+01
    1000.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      21421.391
-3.435135370D+05-2.420680834D+02 1.618029250D+01-7.193817680D-05 1.585712708D-08
-1.814017733D-12 8.388391180D-17      -2.339658121D+05-5.233898700D+01

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## Appendix D (continued)

KBO2                      Gurvich,1982 pt1 p415 pt2 p439.

2 tps82 K	1.00B	1.000	2.00	0.00	0.00	0	81.9081000	-668023.297
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.296308650D+04	-7.209616430D+02	8.349639350D+00	2.407820401D-03	-1.680003427D-07				
-1.231930486D-09	5.479951640D-13		-7.868523470D+04	-1.476077068D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.890726600D+04	-1.671432436D+03	1.117483930D+01	-4.513760260D-04	9.699003460D-08				
-1.090027690D-11	4.976845800D-16		-7.375336080D+04	-3.274749370D+01				

KBr                      Gurvich,1982 pt1 p396 pt2 p423.

2 tps82 K	1.00BR	1.00	0.00	0.00	0.00	0	119.0023000	-179250.878
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.203309190D+03	-2.137880361D+02	5.588509150D+00	-2.753854319D-03	4.013672610D-06				
-2.856323127D-09	8.135209740D-13		-2.188387013D+04	-1.707501588D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.562614367D+06	-4.384894780D+03	9.045464600D+00	-2.045680900D-03	4.401923850D-07				
-1.448178289D-11	-2.273338760D-15		5.315342010D+03	-2.864647026D+01				

KCN                      Chase,1998 p620.

2 j 3/66 K	1.00C	1.00N	1.00	0.00	0.00	0	65.1157000	79496.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.798627669D+04	-6.300558970D+02	9.988695000D+00	-1.076486132D-02	1.751014980D-05				
-1.265592431D-08	3.469762810D-12		1.058025371D+04	-2.594060289D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.615663870D+05	-1.749018011D+03	8.680702670D+00	-4.402350040D-04	9.249499710D-08				
-1.021916855D-11	4.604767190D-16		1.813734856D+04	-2.281619241D+01				

KCL                      Gurvich,1982 pt1 p393 pt2 p420.

2 tps82 K	1.00CL	1.00	0.00	0.00	0.00	0	74.5513000	-214574.881
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.058351510D+03	-2.456801212D+02	5.680696190D+00	-2.900127425D-03	4.130983060D-06				
-2.907340629D-09	8.223850870D-13		-2.597304884D+04	-3.677976854D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.122945722D+05	9.346158900D+02	2.866264958D+00	1.468386693D-03	-5.834260780D-07				
1.255777709D-10	-9.150148000D-15		-3.273787640D+04	1.401864636D+01				

KF                      Gurvich,1982 pt1 p389 pt2 p417.

2 tps82 K	1.00F	1.00	0.00	0.00	0.00	0	58.0967032	-328444.886
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.435704906D+04	-3.391848230D+02	5.727906720D+00	-2.518371562D-03	3.265915640D-06				
-2.210110860D-09	6.212042050D-13		-3.914254420D+04	-5.810999620D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.483743237D+06	4.550048040D+03	-1.081464319D+00	3.503965880D-03	-1.093902537D-06				
1.771028824D-10	-1.029032783D-14		-6.963329810D+04	4.088635920D+01				

KH                      Gurvich,1982 pt1 p383 pt2 p412.

2 tps82 K	1.00H	1.00	0.00	0.00	0.00	0	40.1062400	125399.106
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.237782150D+02	-1.793554623D+02	1.130735415D+00	9.966112560D-03	-1.341218171D-05				
9.034529940D-09	-2.409887770D-12		1.338250358D+04	1.552739897D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.752276520D+06	1.172778444D+04	-1.014137678D+01	8.854548900D-03	-2.517188074D-06				
3.344072360D-10	-1.701157835D-14		-6.025103300D+04	1.010304590D+02				

KI                      Gurvich,1982 pt1 p400 pt2 p426.

2 tps82 K	1.00I	1.00	0.00	0.00	0.00	0	166.0027700	-128455.877
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.572811740D+02	-6.331769730D+01	4.823292420D+00	-7.876668320D-04	1.336737911D-06				
-1.000530992D-09	3.004503956D-13		-1.650340769D+04	3.552594820D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.293747780D+06	-1.002824194D+04	1.629302044D+01	-6.696396750D-03	2.001412089D-06				
-2.677673023D-10	1.273359646D-14		4.676348670D+04	-7.859123370D+01				

KLi                      Gurvich,1982 pt1 p419 pt2 p444.

2 tps82 K	1.00LI	1.00	0.00	0.00	0.00	0	46.0393000	170702.323
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.426043690D+03	-1.986063081D+01	4.487607050D+00	5.249535550D-04	-1.207990165D-06				
1.705161047D-09	-7.879994210D-13		1.927868247D+04	1.912285942D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.211296843D+07	-4.081004870D+04	5.683792120D+01	-3.128695515D-02	8.975062200D-06				
-1.189303691D-09	5.880129180D-14		2.738792595D+05	-3.669693600D+02				

## Appendix D (continued)

KNO<sub>2</sub> Gurvich,1982 pt1 p406 pt2 p431.  
 2 tpis82 K 1.00N 1.000 2.00 0.00 0.00 0 85.1038000 -192497.394  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15342.606  
 -7.246236930D+04 1.226722811D+03-2.258926457D+00 3.019643903D-02-3.640259950D-05  
 2.219135205D-08-5.471654230D-12 -3.077268960D+04 4.537172549D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15342.606  
 -1.689414093D+05-8.515973150D+02 1.063209586D+01-2.523254810D-04 5.573644410D-08  
 -6.393185920D-12 2.964484049D-16 -2.187701436D+04-2.755200432D+01

KNO<sub>3</sub> Gurvich,1982 pt1 p409 pt2 p433.  
 2 tpis82 K 1.00N 1.000 3.00 0.00 0.00 0 101.1032000 -315832.888  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15917.112  
 -2.596112303D+04 8.200606610D+02-2.886015624D+00 4.207288900D-02-5.270323090D-05  
 3.308561730D-08-8.365860370D-12 -4.335054470D+04 4.603187331D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15917.112  
 -3.183682870D+05-1.375234449D+03 1.401587531D+01-4.040660080D-04 8.900847780D-08  
 -1.018771993D-11 4.715982020D-16 -3.513853220D+04-4.804256439D+01

KNa Gurvich,1982 pt1 p420 pt2 p445.  
 2 tpis82 K 1.00NA 1.00 0.00 0.00 0.00 0 62.0880700 132404.327  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10574.127  
 2.542405292D+04-4.119207410D+02 6.841087950D+00-6.250481380D-03 8.861013140D-06  
 -4.922415350D-09 6.493212470D-13 1.652599890D+04-9.136166910D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10574.127  
 6.260326620D+06-2.563593614D+04 4.373335450D+01-2.672655110D-02 8.232705790D-06  
 -1.128503590D-09 5.663264890D-14 1.697274909D+05-2.664117219D+02

KO Gurvich,1982 pt1 p375 pt2 p404.  
 2 tpis82 K 1.000 1.00 0.00 0.00 0.00 0 55.0977000 64733.314  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9481.114  
 1.462562908D+04-3.384765650D+02 5.716607640D+00-2.363265083D-03 2.848716276D-06  
 -1.739858233D-09 4.431006520D-13 8.141835380D+03-4.022101520D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9481.114  
 6.960103380D+05-3.304835290D+03 1.005743444D+01-4.331112000D-03 1.747281632D-06  
 -3.012370548D-10 1.790827870D-14 2.604972496D+04-3.448781520D+01

KOH Gurvich,1997.  
 2 g 9/97 K 1.000 1.00H 1.00 0.00 0.00 0 56.1056400 -232000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11674.650  
 1.770684196D+04-6.153205220D+02 8.684075720D+00-3.962849510D-03 3.408650590D-06  
 -9.601972220D-10 8.494054970D-15 -2.677903261D+04-2.174495666D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11674.650  
 8.917271950D+05-2.334179072D+03 7.972578710D+00 1.038863156D-04-6.315893470D-08  
 1.027938106D-11-5.736685820D-16 -1.443696469D+04-2.076401416D+01

K<sub>2</sub> Gurvich,1982 pt1 p370 pt2 p402.  
 2 tpis82 K 2.00 0.00 0.00 0.00 0.00 0 78.1966000 126546.329  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10741.129  
 1.524169293D+04-3.301789360D+02 7.070795950D+00-9.767072460D-03 2.021535863D-05  
 -1.886092452D-08 6.112974640D-12 1.533402849D+04-9.101035800D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10741.129  
 -2.734470745D+07 6.562180010D+04-4.476350440D+01 8.938859150D-03 2.984557092D-06  
 -1.064158914D-09 8.334936930D-14 -4.226243830D+05 3.867142510D+02

K<sub>2</sub>+ Gurvich,1982 pt1 p374 pt2 p403.  
 2 tpis82 K 2.00E -1.00 0.00 0.00 0.00 0 78.1960514 524660.731  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10861.131  
 5.196036570D+04-6.113382530D+02 7.264990540D+00-5.810634820D-03 6.567496500D-06  
 -2.378020865D-09-1.318637581D-13 6.479820270D+04-1.042370517D+01  
 1000.000 3000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10861.131  
 1.107950739D+07-4.177483820D+04 6.448659840D+01-4.024998030D-02 1.360587923D-05  
 -2.361920107D-09 1.673430610D-13 3.177612050D+05-4.105063100D+02

K<sub>2</sub>Br<sub>2</sub> Gurvich,1982 pt1 p397 pt2 p424.  
 2 tpis82 K 2.00BR 2.00 0.00 0.00 0.00 0 238.0046000 -538744.193  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20951.806  
 -1.093040504D+04-4.856651480D+01 1.019754923D+01-4.363157100D-04 5.387173660D-07  
 -3.486116500D-10 9.190702950D-14 -6.758073240D+04-1.294944706D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20951.806  
 -1.589229976D+04-8.101379460D-01 1.000069442D+01-3.074491521D-07 7.331024160D-11  
 -8.908944780D-15 4.319245430D-19 -6.782595440D+04-1.180425726D+01

## Appendix D (continued)

K2CO3                      Gurvich,1982 pt1 p411 pt2 p435.  
 2 tpis82 K    2.00C    1.000    3.00    0.00    0.00 0    138.2055000    -811649.163  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    19515.837  
 -4.407406700D+04 7.069815440D+02 6.931482470D-01 3.967831320D-02-4.850958300D-05  
 2.976635787D-08-7.374761530D-12                      -1.033913232D+05 2.980651689D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    19515.837  
 -3.264263160D+05-1.521168973D+03 1.712283562D+01-4.464580710D-04 9.833379630D-08  
 -1.125478371D-11 5.210069120D-16                      -9.488275100D+04-6.215220630D+01

K2C2N2                      Chase,1998 p678.  
 2 j 3/66 K    2.00C    2.00N    2.00    0.00    0.00 0    130.2314000    -8368.000  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    24786.242  
 4.627789480D+03-9.729810620D+02 1.996665910D+01-1.953015081D-02 3.275330460D-05  
 -2.393985120D-08 6.596548240D-12                      -7.774411260D+02-6.755613632D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    24786.242  
 7.269599500D+05-3.492108680D+03 1.835676822D+01-8.785475140D-04 1.845532919D-07  
 -2.038717568D-11 9.185420990D-16                      1.582600773D+04-6.728484052D+01

K2CL2                      Gurvich,1982 pt1 p393 pt2 p421.  
 2 tpis82 K    2.00CL    2.00    0.00    0.00    0.00 0    149.1026000    -615393.663  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    19963.448  
 -1.328526456D+04-1.241832429D+02 1.050035730D+01-1.097776004D-03 1.348871402D-06  
 -8.697215120D-10 2.286584080D-13                      -7.644363150D+04-1.790150052D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    19963.448  
 -2.614611331D+04-2.096229095D+00 1.000178456D+01-7.864803710D-07 1.869281152D-10  
 -2.266272348D-14 1.096790704D-18                      -7.707189330D+04-1.499720802D+01

K2F2                      Gurvich,1982 pt1 p389 pt2 p418.  
 2 tpis82 K    2.00F    2.00    0.00    0.00    0.00 0    116.1934064    -859875.481  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18125.626  
 -1.611833856D+03-5.135644890D+02 1.199922511D+01-4.280109550D-03 5.165387540D-06  
 -3.285814900D-09 8.549648750D-13                      -1.039248602D+05-3.039925079D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18125.626  
 -5.740892530D+04-9.046182110D+00 1.000750685D+01-3.250764840D-06 7.630064590D-10  
 -9.165649530D-14 4.405048440D-18                      -1.065413546D+05-1.874037620D+01

K2I2                      Gurvich,1982 pt1 p401 pt2 p427.  
 2 tpis82 K    2.00I    2.00    0.00    0.00    0.00 0    332.0055400    -418915.452  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    21456.548  
 -8.977752440D+03-2.776460169D+01 1.011331014D+01-2.508421994D-04 3.102352114D-07  
 -2.010096209D-10 5.304437150D-14                      -5.326208390D+04-1.032092509D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    21456.548  
 -1.179634729D+04-4.724761550D-01 1.000040695D+01-1.807689054D-07 4.320560970D-11  
 -5.259699430D-15 2.553419144D-19                      -5.340210230D+04-9.664440500D+00

K2O                      Gurvich,1982 pt1 p377 pt2 p407.  
 2 tpis82 K    2.00O    1.00    0.00    0.00    0.00 0    94.1960000    -74086.902  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13858.298  
 2.392044068D+04-5.445358390D+02 8.826403230D+00-3.481429430D-03 3.834542070D-06  
 -2.268494189D-09 5.569212250D-13                      -8.234291680D+03-1.663099064D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    13858.298  
 -4.611464580D+04-1.363119524D+01 7.010530440D+00-4.323658260D-06 9.747788420D-10  
 -1.135283694D-13 5.325860600D-18                      -1.107222244D+04-5.768718720D+00

K2O+                      Gurvich,1982 pt1 p379 pt2 p408.  
 2 tpis82 K    2.00O    1.00E -1.00    0.00    0.00 0    94.1954514    368390.321  
   298.150    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14138.121  
 7.201102730D+03-3.336526400D+02 8.050730350D+00-1.869353797D-03 1.921291874D-06  
 -1.064020951D-09 2.457514799D-13                      4.389986360D+04-1.073204150D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    14138.121  
 -3.780033500D+04-8.849537390D+00 7.006847890D+00-2.815510856D-06 6.355001500D-10  
 -7.408551990D-14 3.478334960D-18                      4.214519680D+04-4.418276610D+00

K2O2                      Gurvich,1982 pt1 p381 pt2 p410.  
 2 tpis82 K    2.00O    2.00    0.00    0.00    0.00 0    110.1954000    -191566.301  
   200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    16289.803  
 4.810870610D+04-1.003601504D+03 1.154229002D+01-4.546332520D-04-1.516606209D-06  
 1.799426090D-09-6.128337290D-13                      -2.057151920D+04-3.181199790D+01  
   1000.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    16289.803  
 -1.476073073D+05-1.021932040D+02 1.007664713D+01-3.076517991D-05 6.815252810D-09  
 -7.828654450D-13 3.632506100D-17                      -2.592056324D+04-2.162287184D+01

## Appendix D (continued)

K2O2H2                      Gurvich, 1997.

2 g 9/97 K	2.000	2.00H	2.00	0.00	0.00	0	112.2112800	-641000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
8.174788370D+03	-1.130630680D+03	1.815303256D+01	-7.737431080D-03	6.837614010D-06				
-2.054691111D-09	7.672877510D-14		-7.574965170D+04	-6.391759470D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
1.773523196D+06	-4.665292470D+03	1.694308128D+01	2.085297143D-04	-1.264714762D-07				
2.057506565D-11	-1.148042134D-15		-5.051263310D+04	-6.334773920D+01				

K2SO4                      Gurvich, 1982 pt1 p404 pt2 p429.

2 g10/99 K	2.00S	1.000	4.00	0.00	0.00	0	174.2592000	-1095851.121
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
6.271492310D+04	-8.152049920D+02	7.455413720D+00	3.849909780D-02	-5.400630980D-05				
3.654656800D-08	-9.760223570D-12		-1.304692568D+05	-1.034634770D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-5.446125640D+05	-9.590667230D+02	1.971591285D+01	-2.866586009D-04	6.342480640D-08				
-7.281462540D-12	3.377886930D-16		-1.337873384D+05	-7.399103551D+01				

Kr                      Ref-Elm. Sugar, 1991.

3 g 8/97 KR	1.00	0.00	0.00	0.00	0.00	0	83.8000000	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
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	5.490956510D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
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
-1.375531087D+09	9.064030530D+05	-2.403481435D+02	3.378312030D-02	-2.563103877D-06				
9.969787790D-11	-1.521249677D-15		-7.111667370D+06	2.086866326D+03				

Kr+                      Sugar, 1991. Gordon, 1999.

3 g 7/97 KR	1.00E	-1.00	0.00	0.00	0.00	0	83.7994514	1356953.918
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-5.650402860D+03	6.930740810D+01	2.157028132D+00	8.711228930D-04	-1.181609730D-06				
7.862198630D-10	-1.832589387D-13		1.621164118D+05	8.818242260D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-2.216567015D+05	1.166167840D+03	4.869655320D-01	1.429223599D-03	-3.949628610D-07				
4.982853510D-11	-2.406719258D-15		1.556002861D+05	2.059230986D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-3.319875960D+07	1.797953100D+04	-7.155015940D-01	2.671088984D-04	-6.196251880D-09				
-4.107025960D-13	2.000619351D-17		1.648114259D+04	3.620325750D+01				

Li                      Hf: Cox, 1989. Moore, 1971. Gordon, 1999.

3 g 7/97 LI	1.00	0.00	0.00	0.00	0.00	0	6.9410000	159300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		1.841390197D+04	2.447622965D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
1.125610652D+06	-3.463536730D+03	6.566611920D+00	-2.260983356D-03	5.922289160D-07				
-6.281635100D-11	2.884948238D-15		4.034637400D+04	-2.655918195D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
2.604352623D+09	-1.521952201D+06	3.454400500D+02	-3.779674850D-02	2.222420069D-06				
-6.691570800D-11	8.088023606D-16		1.217791847D+07	-3.006680193D+03				

Li+                      Moore, 1971. Gordon, 1999.

3 g 3/97 LI	1.00E	-1.00	0.00	0.00	0.00	0	6.9404514	685719.428
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		8.172724550D+04	1.754357228D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		8.172724550D+04	1.754357228D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		8.172724550D+04	1.754357228D+00				

## Appendix D (continued)

Li- Hotop,1985. Gordon,1999.

3 g 1/98 LI	1.00E	1.00	0.00	0.00	0.00	0.00	0.00	6.9415486	93474.728
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							1.049698659D+04	1.754594332D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							1.049698659D+04	1.754594332D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							1.049698659D+04	1.754594332D+00

LiAlF4 Gurvich,1982 pt1 p300 pt2 p333.

2 tps82 LI	1.00AL	1.00F	4.00	0.00	0.00	0	109.9161508	-1857287.824
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.761529360D+05	-2.999300134D+03	2.079739570D+01	-1.742914656D-03	-4.266642090D-06				
5.362829770D-09	1.866817087D-12							-2.117947828D+05
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.020700930D+05	-2.783355146D+02	1.620791185D+01	-8.316341570D-05	1.836905690D-08				
-2.104932808D-12	9.747253020D-17							-2.278696416D+05

LiBO2 Gurvich,1982 pt1 p299 pt2 p332.

2 tps82 LI	1.00B	1.00O	2.00	0.00	0.00	0	49.7508000	-652352.276
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.518987570D+04	-1.060320845D+03	9.548049960D+00	-5.469576070D-05	2.658687599D-06				
-2.931603694D-09	9.663029730D-13							-7.506204110D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.554404520D+04	-1.731920898D+03	1.121462090D+01	-4.659162170D-04	9.999875690D-08				
-1.122880592D-11	5.123529460D-16							-7.154743820D+04

LiBr Gurvich,1982 pt1 p285 pt2 p318.

2 tps82 LI	1.00BR	1.00	0.00	0.00	0.00	0	86.8450000	-151162.890
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.805620470D+04	-6.129614990D+02	6.577369550D+00	-4.219891760D-03	5.391423370D-06				
-3.693144810D-09	1.049158761D-12							-1.637487617D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.380191420D+04	-2.597050764D+02	4.656768870D+00	1.022867706D-04	-5.178252340D-08				
2.058203991D-11	-1.942190308D-15							-1.793363752D+04

LiCl Gurvich,1982 pt1 p281 pt2 p314.

2 tps82 LI	1.00CL	1.00	0.00	0.00	0.00	0	42.3940000	-193779.891
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.964399500D+04	-7.187346620D+02	6.785147030D+00	-4.522145460D-03	5.748483700D-06				
-3.966255670D-09	1.137911398D-12							-2.091014703D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.352769705D+05	6.120046920D+02	3.634293730D+00	6.810973320D-04	-2.174238799D-07				
4.220403610D-11	-2.848628426D-15							-2.862358494D+04

LiF Gurvich,1982 pt1 p275 pt2 p310.

2 tps89 LI	1.00F	1.00	0.00	0.00	0.00	0	25.9394032	-340944.894
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.912537320D+04	-2.531413159D+02	3.539727980D+00	3.695917040D-03	-4.829466150D-06				
2.944090711D-09	-6.838794740D-13							-4.064849660D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.784246490D+05	7.668062460D+02	3.585473400D+00	6.031084350D-04	-1.588764206D-07				
2.569397177D-11	-1.406798386D-15							-4.756469450D+04

LiH Gurvich,1982 pt1 p265 pt2 p301.

2 tps82 LI	1.00H	1.00	0.00	0.00	0.00	0	7.9489400	139264.104
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.913731570D+04	7.756092190D+02	-1.011102377D+00	1.145479597D-02	-1.151038734D-05				
5.875068960D-09	-1.196789735D-12							1.204858910D+04
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.633686357D+06	6.996429170D+03	-3.233533060D+00	4.033935980D-03	-9.099579640D-07				
8.775909870D-11	-2.889490251D-15							-2.990043016D+04

LiI Gurvich,1982 pt1 p289 pt2 p322.

2 tps82 LI	1.00I	1.00	0.00	0.00	0.00	0	133.8454700	-85269.888
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.071976370D+04	-6.667289470D+02	7.064257530D+00	-5.480041020D-03	6.905790160D-06				
-4.537168520D-09	1.226373296D-12							-8.235487020D+03
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.616342632D+06	-4.877717080D+03	9.987186550D+00	-2.889137815D-03	8.037313770D-07				
-9.028172610D-11	3.078321954D-15							1.937718764D+04



## Appendix D (continued)

LiN Chase, 1998 p1500.

2 j12/66 LI	1.00N	1.00	0.00	0.00	0.00	0.00	0.00	20.9477000	334720.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0
3.764959200D+04	-4.883457630D+02	5.187373450D+00	2.275252171D-04	-1.416337564D-06					
1.450236258D-09	-4.790014330D-13		4.161915310D+04	-5.952157244D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.993489980D+04	-4.031134550D+01	4.529624210D+00	8.744156930D-05	2.557428364D-09					
-2.905751800D-13	1.336125922D-17		3.894831130D+04	-1.214952896D+00					

LiNO2 Gurvich, 1982 pt1 p294 pt2 p327.

2 tpis82 LI	1.00N	1.000	2.00	0.00	0.00	0	52.9465000	-202031.208
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
-3.133773859D+04	5.389940810D+02	-2.059877081D-02	2.610777454D-02	-3.209235040D-05				
1.974344044D-08	-4.892199160D-12		-2.838214963D+04	2.710019529D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.196671160D+05	-8.610042710D+02	1.063956465D+01	-2.554392587D-04	5.644478540D-08				
-6.476140050D-12	3.003536591D-16		-2.313547535D+04	-3.238277103D+01				

LiNO3 Gurvich, 1982 pt1 p296 pt2 p329.

2 tpis82 LI	1.00N	1.000	3.00	0.00	0.00	0	68.9459000	-311584.675
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
1.967205518D+04	9.052795260D+01	-5.109770400D-01	3.756605950D-02	-4.782738650D-05				
3.029277805D-08	-7.708013150D-12		-3.907563990D+04	2.746873033D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.559402450D+05	-1.447644737D+03	1.406684061D+01	-4.236371280D-04	9.320824510D-08				
-1.065894872D-11	4.930780620D-16		-3.434827460D+04	-5.275382697D+01				

LiO Gurvich, 1982 pt1 p256 pt2 p294.

2 tpis82 LI	1.000	1.00	0.00	0.00	0.00	0	22.9404000	72914.313
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
3.627029760D+04	-3.499363230D+02	4.394933180D+00	1.079712984D-03	-8.724033810D-07				
5.607962970D-10	-2.054288457D-13		9.533330530D+03	-9.058149610D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.612392133D+06	-5.551312340D+03	1.120573851D+01	-3.437226880D-03	9.133194660D-07				
-1.027902258D-10	3.822991000D-15		4.201575470D+04	-4.857354580D+01				

LiOF Chase, 1998 p1069.

2 j 9/65 LI	1.000	1.00F	1.00	0.00	0.00	0	41.9388032	-92048.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
5.510110690D+04	-5.770688170D+02	4.424954930D+00	1.102425422D-02	-1.710493381D-05				
1.234361201D-08	-3.453693000D-12		-9.278986980D+03	1.238830687D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.833563281D+05	-2.110049301D+02	7.156818170D+00	-6.249462010D-05	1.376567002D-08				
-1.574099067D-12	7.277167140D-17		-1.254530277D+04	-1.272130479D+01				

LiOH Gurvich, 1996b.

2 g12/96 LI	1.000	1.00H	1.00	0.00	0.00	0	23.9483400	-229000.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
4.574190120D+03	-1.030949027D+02	4.272407370D+00	8.465219230D-03	-1.386148524D-05				
1.101099795D-08	-3.291248210D-12		-2.848728855D+04	-8.775745780D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
8.500751370D+05	-2.430540791D+03	8.055314620D+00	6.895680880D-05	-5.527207460D-08				
9.368054030D-12	-5.313785680D-16		-1.365894396D+04	-2.457598093D+01				

LiON Chase, 1998 p1501.

2 j 9/66 LI	1.000	1.00N	1.00	0.00	0.00	0	36.9471000	179912.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
-9.412672670D+03	1.009332300D+02	3.006187607D+00	9.890462200D-03	-1.128294343D-05				
6.410291740D-09	-1.466806373D-12		1.978348318D+04	1.016334813D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.740629140D+04	-5.111560940D+02	7.378493870D+00	-1.508777884D-04	3.329914980D-08				
-3.817514290D-12	1.769558455D-16		2.211006635D+04	-1.454105040D+01				

Li2 Chase, 1998 p1505.

2 j12/83 LI	2.00	0.00	0.00	0.00	0.00	0	13.8820000	215900.000
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0
6.778481580D+03	-2.246205832D+02	5.296037440D+00	-1.272412017D-03	1.205843729D-06				
-9.818544590D-11	-2.416702607D-13		2.573638186D+04	-6.869257580D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.767645400D+07	-1.185747185D+05	1.482167789D+02	-8.378532110D-02	2.424919798D-05				
-3.275820240D-09	1.652000081D-13		7.723072010D+05	-1.021697298D+03				

## Appendix D (continued)

Li2+ Gurvich,1982 pt1 p249 pt2 p292.

2	tpis82	LI	2.00E	-1.00	0.00	0.00	0.00	0	13.8814514	721611.420
298.150	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.040056453D+04	2.675405642D+01	4.247271750D+00	1.057450777D-03	-1.281715096D-06						
1.067477239D-09	-2.759413508D-13		8.529811310D+04	5.298189960D-01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9989.120
1.279931073D+07	-3.492861390D+04	3.844785360D+01	-1.380635397D-02	2.531394250D-06						
-2.197815991D-10	7.087669250D-15		3.117964450D+05	-2.509543641D+02						

Li2Br2 Gurvich,1982 pt1 p286 pt2 p319.

2	tpis82	LI	2.00BR	2.00	0.00	0.00	0.00	0	173.6900000	-495833.524
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
2.786312863D+04	-1.005641437D+03	1.370963066D+01	-7.633663300D-03	8.942905920D-06						
-5.561135090D-09	1.421736784D-12		-5.762845840D+04	-4.121843760D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16950.476
-8.900983360D+04	-1.988916335D+01	1.001596418D+01	-6.749134050D-06	1.556299963D-09						
-1.8446930258D-13	8.774879920D-18		-6.279989960D+04	-1.943063525D+01						

Li2CL2 Gurvich,1982 pt1 p282 pt2 p315.

2	tpis82	LI	2.00CL	2.00	0.00	0.00	0.00	0	84.7880000	-597538.789
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
5.313398610D+04	-1.427266759D+03	1.512410161D+01	-1.032824906D-02	1.190773317D-05						
-7.312991160D-09	1.851289430D-12		-6.769860400D+04	-5.285131549D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	15906.322
-1.179571272D+05	-3.027126342D+01	1.002397711D+01	-1.003660907D-05	2.297007564D-09						
-2.706930258D-13	1.281817017D-17		-7.506822590D+04	-2.264970230D+01						

Li2F2 Gurvich,1982 pt1 p276 pt2 p311.

2	tpis82	LI	2.00F	2.00	0.00	0.00	0.00	0	51.8788064	-935323.076
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
1.443166185D+05	-2.466874678D+03	1.702863290D+01	-1.145541210D-02	1.086098792D-05						
-5.569754280D-09	1.193819664D-12		-1.026070133D+05	-7.000386610D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13766.030
-2.188931683D+05	-9.259814530D+01	1.006970757D+01	-2.803632163D-05	6.217549520D-09						
-7.146267020D-13	3.316857300D-17		-1.156611527D+05	-2.729853181D+01						

Li2I2 Gurvich,1982 pt1 p290 pt2 p323.

2	tpis82	LI	2.00I	2.00	0.00	0.00	0.00	0	267.6909400	-362801.349
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
1.014872266D+04	-7.120421010D+02	1.270392960D+01	-5.685536810D-03	6.770340380D-06						
-4.263304890D-09	1.100658186D-12		-4.313063860D+04	-3.303950980D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	17658.652
-6.973587060D+04	-1.316825508D+01	1.001074855D+01	-4.600203780D-06	1.070510527D-09						
-1.277717768D-13	6.110612240D-18		-4.677470050D+04	-1.721894034D+01						

Li2O Gurvich,1982 pt1 p259 pt2 p296.

2	tpis82	LI	2.00O	1.00	0.00	0.00	0.00	0	29.8814000	-167338.920
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
2.636601597D+04	-1.798629279D+02	4.051115220D+00	1.189981375D-02	-1.730095793D-05						
1.205584550D-08	-3.292733880D-12		-2.061907963D+04	1.605995610D+00						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	12792.080
7.261487040D+05	-9.543783720D+03	2.887491643D+01	-1.959494099D-02	8.086339840D-06						
-1.370211764D-09	8.111727190D-14		2.990726399D+04	-1.564517822D+02						

Li2O+ Gurvich,1982 pt1 p260 pt2 p297.

2	tpis82	LI	2.00O	1.00E	-1.00	0.00	0.00	0	29.8808514	439095.089
298.150	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
1.081044623D+05	-1.261961355D+03	9.692011290D+00	-1.793477428D-03	3.380326900D-07						
4.143395150D-10	-1.990530222D-13		5.754976040D+04	-2.915719946D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13028.689
-1.302166086D+05	-1.466759528D+02	7.610729450D+00	-4.469426690D-05	9.947160640D-09						
-1.147038806D-12	5.339241470D-17		5.098762310D+04	-1.528011047D+01						

Li2O2 Gurvich,1982 pt1 p262 pt2 p299.

2	tpis82	LI	2.00O	2.00	0.00	0.00	0.00	0	45.8808000	-279397.988
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13548.012
1.392619730D+05	-1.764036747D+03	1.029649198D+01	7.605949950D-03	-1.538519312D-05						
1.238199941D-08	-3.685431570D-12		-2.638056746D+04	-3.437710560D+01						
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13548.012
-2.939232153D+05	-2.359107937D+02	1.017463402D+01	-6.931624360D-05	1.521202834D-08						
-1.733841909D-12	7.993154620D-17		-3.618481910D+04	-2.904221044D+01						

## Appendix D (continued)

Li2O2H2 Gurvich, 1996b.

2 g12/96 LI	2.000	2.00H	2.00	0.00	0.00	0	47.8966800	-737000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.894413579D+05	-2.779117524D+03	1.530234911D+01	1.070738317D-02	-2.510075145D-05				
2.224910575D-08	-6.949359580D-12		-7.702776920D+04	-6.514116940D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.215377492D+06	-3.982057440D+03	1.585877373D+01	7.509145680D-04	-2.585218184D-07				
3.646841700D-11	-1.904139406D-15		-6.738748380D+04	-6.647208400D+01				

Li2SO4 Chase, 1998 p1522.

2 j12/78 LI	2.00S	1.000	4.00	0.00	0.00	0	109.9446000	-1041816.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.006318702D+05	-1.543457217D+03	9.670054910D+00	3.390757380D-02	-4.823483810D-05				
3.267368920D-08	-8.702518510D-12		-1.201939538D+05	-2.911716635D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.038750870D+05	-1.064550976D+03	1.979557349D+01	-3.188978250D-04	7.062411120D-08				
-8.114439070D-12	3.766830210D-16		-1.268908595D+05	-8.014316674D+01				

Li3+ Gurvich, 1982 pt1 p251 pt2 p293.

2 tpis82 LI	3.00E	-1.00	0.00	0.00	0.00	0	20.8224514	756590.836
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.87322290D+03	-2.820780467D+02	7.922697480D+00	-1.687949474D-03	1.771718993D-06				
-9.972535400D-10	2.332934849D-13		9.027963650D+04	-1.619319856D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.355098060D+04	-6.056432750D+00	7.004722890D+00	-1.953320933D-06	4.429152230D-10				
-5.181983190D-14	2.439894871D-18		8.879902870D+04	-1.066880792D+01				

Li3Br3 Gurvich, 1982 pt1 p287 pt2 p320.

2 tpis82 LI	3.00BR	3.00	0.00	0.00	0.00	0	260.5350000	-824639.193
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.431966250D+04	-1.823743601D+03	2.243492856D+01	-1.279418260D-02	1.459200355D-05				
-8.884688150D-09	2.233708050D-12		-9.480677670D+04	-8.206864420D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.584670201D+05	-4.041360940D+01	1.603177633D+01	-1.322713911D-05	3.014221791D-09				
-3.540292160D-13	1.672030783D-17		-1.042470448D+05	-4.405478160D+01				

Li3CL3 Gurvich, 1982 pt1 p283 pt2 p316.

2 tpis82 LI	3.00CL	3.00	0.00	0.00	0.00	0	127.1820000	-976107.121
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.867429000D+04	-2.324074851D+03	2.378484564D+01	-1.483522400D-02	1.634495612D-05				
-9.675366520D-09	2.377033859D-12		-1.103839177D+05	-9.474114379D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.005930356D+05	-5.939400190D+01	1.604590929D+01	-1.885890854D-05	4.253517370D-09				
-4.955560940D-13	2.325408214D-17		-1.224927071D+05	-4.844413629D+01				

Li3F3 Gurvich, 1982 pt1 p278 pt2 p312.

2 tpis82 LI	3.00F	3.00	0.00	0.00	0.00	0	77.8182096	-1524596.926
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.823874443D+05	-3.163786240D+03	2.287811928D+01	-7.544903890D-03	3.446790230D-06				
2.690705228D-10	-5.250840960D-13		-1.712446093D+05	-9.973654990D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.618664990D+05	-1.937051395D+02	1.614457133D+01	-5.775628500D-05	1.274057038D-08				
-1.458168875D-12	6.744850030D-17		-1.882081974D+05	-5.633612880D+01				

Li3I3 Gurvich, 1982 pt1 p290 pt2 p324.

2 tpis82 LI	3.00I	3.00	0.00	0.00	0.00	0	401.5364100	-612457.307
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.611764690D+04	-1.392033487D+03	2.110791892D+01	-1.046866587D-02	1.222589173D-05				
-7.584135430D-09	1.935199180D-12		-7.153084580D+04	-7.093882030D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.266696511D+05	-2.783891914D+01	1.602228068D+01	-9.399364930D-06	2.163919735D-09				
-2.561731922D-13	1.217394107D-17		-7.869550680D+04	-4.091724060D+01				

Mg Hf:Cox, 1989. Kaufman, 1991a. Gordon, 1999.

3 g 6/97 MG	1.00	0.00	0.00	0.00	0.00	0	24.3050000	147100.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		1.694658761D+04	3.634330140D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.364831550D+05	1.973709576D+03	-3.633776900D-01	2.071795561D-03	-7.738051720D-07				
1.359277788D-10	-7.766898397D-15		4.829188110D+03	2.339104998D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.166012586D+09	-1.008355665D+06	1.619680021D+02	-8.790130350D-03	-1.925690961D-08				
1.725045214D-11	-4.234946112D-16		8.349525900D+06	-1.469355261D+03				

## Appendix D (continued)

Mg+ Kaufman, 1991a. Gordon, 1999.

3 g 6/97 MG	1.00E	-1.00	0.00	0.00	0.00	0.00	0.00	24.3044514	891047.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00							1.064223354D+05	4.327443460D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.914758821D+04	4.877347920D+01	2.457662661D+00	1.218104674D-05	1.897261686D-09					
-1.580433756D-12	2.135732238D-16							1.061022394D+05	4.646442860D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.015949550D+08	-2.281591735D+05	5.421745710D+01	-5.983017190D-03	3.657189130D-07					
-1.020737688D-11	1.024202854D-16							1.932463961D+06	-4.480157830D+02

MgBr Gurvich, 1996a pt1 p417 pt2 p331.

2 tpis96 MG	1.00BR	1.00	0.00	0.00	0.00	0.00	0.00	104.2090000	6163.315
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.361419140D+03	-2.395789881D+02	5.360560420D+00	-1.667141829D-03	1.981137765D-06					
-1.201637202D-09	3.032148099D-13							5.915634440D+02	-1.421771179D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.477604216D+04	-6.417687520D+02	6.019932090D+00	-1.391004302D-03	6.443330960D-07					
-1.197734078D-10	7.421644240D-15							2.824060334D+03	-6.264439920D+00

MgBr2 Gurvich, 1996a pt1 p420 pt2 p333.

2 tpis96 MG	1.00BR	2.00	0.00	0.00	0.00	0.00	0.00	184.1130000	-306743.219
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.148477999D+04	-5.154528900D+02	9.273258750D+00	-3.470049040D-03	3.921840790D-06					
-2.377174864D-09	5.967025560D-13							-3.652443850D+04	-1.791077763D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.326899010D+04	-1.283036001D+01	7.510024300D+00	-4.152332400D-06	9.426499180D-10					
-1.103873928D-13	5.201104310D-18							-3.919886020D+04	-7.409168030D+00

MgCL Gurvich, 1996a pt1 p412 pt2 p328.

2 tpis96 MG	1.00CL	1.00	0.00	0.00	0.00	0.00	0.00	59.7580000	-54704.887
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.043995280D+04	-4.072155160D+02	5.880372300D+00	-2.594175042D-03	2.945953528D-06					
-1.750648628D-09	4.337959330D-13							-5.851444950D+03	-6.023545750D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.041328453D+06	-3.380158330D+03	8.637775470D+00	-2.447789643D-03	7.841969440D-07					
-1.126409380D-10	5.810620730D-15							1.327188977D+04	-2.703802395D+01

MgCL+ Chase, 1998 p786 6/68.

3 g 1/01 MG	1.00CL	1.00E	-1.00	0.00	0.00	0.00	0.00	59.7574514	646339.332
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.182385120D+03	-2.622253760D+02	5.419863430D+00	-1.774129606D-03	2.185811127D-06					
-1.418143432D-09	3.918898580D-13							7.770403710D+04	-3.780938840D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.268391921D+07	3.478824540D+04	-3.004222950D+01	1.481739497D-02	-2.470965605D-06					
1.424433718D-10	2.789613105D-16							-1.487013740D+05	2.552015117D+02
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.382463416D+08	-6.324735630D+04	2.090164490D+01	-1.924320270D-03	1.303442285D-07					
-4.354246510D-12	5.852012920D-17							5.856144100D+05	-1.379609224D+02

MgCL2 Gurvich, 1996a pt1 p416 pt2 p330.

2 tpis96 MG	1.00CL	2.00	0.00	0.00	0.00	0.00	0.00	95.2110000	-399169.896
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.637824680D+04	-7.307844960D+02	9.661030510D+00	-3.660212940D-03	3.610819350D-06					
-1.928769286D-09	4.309912350D-13							-4.646914570D+04	-2.360112274D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.835217010D+04	-2.490899393D+01	7.518783200D+00	-7.564518260D-06	1.679293770D-09					
-1.931706275D-13	8.971657820D-18							-5.032686910D+04	-1.053268382D+01

MgF Gurvich, 1996a pt1 p408 pt2 p325.

2 tpis96 MG	1.00F	1.00	0.00	0.00	0.00	0.00	0.00	43.3034032	-232266.792
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.823001620D+04	-4.803310390D+02	5.068468940D+00	5.212029300D-04	-1.874026347D-06					
1.759241129D-09	-5.609403190D-13							-2.659114296D+04	-3.768969210D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.695883782D+05	3.588757630D+02	3.936001650D+00	4.813044140D-04	-1.658385409D-07					
3.336052290D-11	-2.270104205D-15							-3.169323990D+04	4.410565900D+00

## Appendix D (continued)

MgF+ Chase,1998 p1071 12/75.

3 g 2/01 MG	1.00F	1.00E	-1.00	0.00	0.00	0	43.3028546	516867.775
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
6.413293840D+05	-8.518532610D+03	4.814216910D+01	-1.163071535D-01	1.622560562D-04				
-1.063484590D-07	2.634809398D-11		1.024308480D+05	-2.450074295D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-1.056852362D+07	2.077122379D+04	-6.119523560D+00	2.245834831D-03	-9.515738610D-08				
-2.263502341D-11	2.284524246D-15		-8.331549880D+04	8.727102380D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
5.735804460D+07	-2.157378345D+04	6.572317550D+00	1.887605214D-04	-1.860864600D-08				
6.862191460D-13	-8.597821080D-18		2.477615733D+05	-1.922750114D+01				

MgF2 Gurvich,1996a pt1 p411 pt2 p327.

2 tpis96 MG	1.00F	2.00	0.00	0.00	0.00	0	62.3018064	-735498.060
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
4.338429550D+04	-6.616511770D+02	7.453448520D+00	3.520814050D-03	-6.955764580D-06				
5.619923480D-09	-1.688028906D-12		-8.687183670D+04	-1.545476790D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-1.244419584D+05	-8.687343750D+01	7.563581230D+00	-2.499267978D-05	5.440129140D-09				
-6.158245760D-13	2.822792666D-17		-9.060019440D+04	-1.420796990D+01				

MgF2+ Chase,1998 p1122 12/75.

3 g 2/01 MG	1.00F	2.00E	-1.00	0.00	0.00	0	62.3012578	582692.164
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
7.832220260D+04	-1.176632752D+03	1.025829767D+01	-3.755272890D-03	3.016621585D-06				
-1.327098871D-09	2.465289749D-13		7.413228550D+04	-2.990883551D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-1.502316870D+05	7.725289560D+01	7.271569360D+00	2.237529770D-04	-1.003070865D-07				
1.996274309D-11	-1.233278721D-15		6.699117500D+04	-1.094528006D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
2.601903911D+07	-5.388879260D+03	5.218198280D+00	7.632535320D-04	-6.606231900D-08				
2.428649361D-12	-3.341900910D-17		1.228640353D+05	3.390783040D+00				

MgH Gurvich,1996a pt1 p401 pt2 p320.

2 tpis96 MG	1.00H	1.00	0.00	0.00	0.00	0	25.3129400	229786.104
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-4.958679150D+04	7.500278650D+02	-6.442047500D-01	9.826301010D-03	-8.789822440D-06				
3.823353520D-09	-6.003725760D-13		2.302279383D+04	2.657165344D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-1.005748598D+05	1.952890106D+03	-1.317191549D+00	5.603665800D-03	-2.137334980D-06				
3.324880500D-10	-1.824672746D-14		1.598582755D+04	3.431233160D+01				

MgI Gurvich,1996a pt1 p420 pt2 p334.

2 tpis96 MG	1.00I	1.00	0.00	0.00	0.00	0	151.2094700	61206.317
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
2.943889099D+03	-1.690248574D+02	5.147251830D+00	-1.321186997D-03	1.623056505D-06				
-1.005114222D-09	2.567337785D-13		6.845890270D+03	8.593132250D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-2.370562811D+06	6.916452480D+03	-3.183894490D+00	4.051551140D-03	-9.774290750D-07				
1.023329400D-10	-3.790304870D-15		-3.818551110D+04	5.993104380D+01				

MgI2 Gurvich,1996a pt1 p423 pt2 p336.

2 tpis96 MG	1.00I	2.00	0.00	0.00	0.00	0	278.1139400	-171706.029
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
1.594739709D+04	-4.160412720D+02	9.010638320D+00	-3.090359024D-03	3.621264260D-06				
-2.260138392D-09	5.809055550D-13		-2.080441400D+04	-1.412175736D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-3.340299180D+04	-9.343511780D+00	7.507468540D+00	-3.147707890D-06	7.241336470D-10				
-8.567664950D-14	4.069691700D-18		-2.294555505D+04	-5.241272590D+00				

MgN Chase,1998 p1535.

2 j 3/64 MG	1.00N	1.00	0.00	0.00	0.00	0	38.3117000	288696.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
3.759538640D+04	-4.853164280D+02	5.163054240D+00	2.591539493D-04	-1.518993975D-06				
1.522840476D-09	-4.992531450D-13		3.607294610D+04	-3.813908776D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								
-6.018589100D+04	-4.010864780D+01	4.529498950D+00	4.760490910D-05	2.547271298D-09				
-2.894058118D-13	1.330639131D-17		3.341285700D+04	7.925250209D-01				

## Appendix D (continued)

MgO Gurvich,1996a pt1 p398 pt2 p318.

3 tpis96 MG	1.000	1.00	0.00	0.00	0.00	0	40.3044000	32261.307
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.513659740D+05	-5.287197160D+03	3.382060060D+01	-8.400489630D-02	1.210016160D-04				
-7.630795020D-08	1.701022862D-11		2.790679519D+04	-1.624886199D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.586738367D+07	3.420468100D+04	-1.774087677D+01	7.004963050D-03	-1.104138249D-06				
8.957488530D-11	3.052513649D-15		-2.300504434D+05	1.738984472D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.290059050D+06	-2.073499632D+04	1.444150005D+01	-1.490609900D-03	1.052119343D-07				
-3.523030610D-12	4.613111760D-17		1.490218815D+05	-8.007281730D+01				

MgOH Gurvich,1996a pt1 p404 pt2 p322.

2 tpis96 MG	1.000	1.00H	1.00	0.00	0.00	0	41.3123400	-132428.980
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.839851620D+04	-7.367383640D+02	7.920664460D+00	-5.950940590D-04	-2.112941162D-06				
3.228282110D-09	-1.214159329D-12		-1.392326188D+04	-1.916078109D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.648664750D+05	-1.770750355D+03	7.269999270D+00	5.336842760D-04	-1.980894443D-07				
3.025677088D-11	-1.554849476D-15		-6.149114560D+03	-1.671027009D+01				

MgOH+ Chase,1998 p1285 12/75.

3 g 1/01 MG	1.000	1.00H	1.00E	-1.00	0.00	0	41.3117914	615769.370
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.170224573D+05	-1.735933343D+03	1.164059613D+01	-8.449876220D-03	7.351713740D-06				
-2.790223071D-09	3.514982130D-13		8.118807670D+04	-4.271174370D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.296339540D+05	-2.459700177D+03	8.118732020D+00	3.500579100D-05	-4.670574750D-08				
8.312358260D-12	-4.802836220D-16		8.801661710D+04	-2.438155217D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.691779770D+06	2.437864449D+03	6.949387850D+00	6.355744850D-05	-3.980850170D-09				
1.287525303D-13	-1.684735436D-18		4.948972630D+04	-1.400323314D+01				

Mg(OH)2 Gurvich,1996a pt1 p407 pt2 p324.

2 tpis96 MG	1.000	2.00H	2.00	0.00	0.00	0	58.3196800	-551995.808
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.245894670D+04	-1.289056383D+03	1.389327642D+01	-7.806693670D-04	-4.151257230D-06				
6.109473040D-09	-2.274138833D-12		-6.295089150D+04	-5.015353340D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.713709254D+06	-4.730005350D+03	1.448925967D+01	1.907819857D-04	-1.226834131D-07				
2.015343753D-11	-1.128993279D-15		-3.887724670D+04	-5.840498120D+01				

MgS Gurvich,1996a pt1 p425 pt2 p338.

2 tpis96 MG	1.00S	1.00	0.00	0.00	0.00	0	56.3700000	120649.311
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.565788090D+03	1.443637798D+02	1.813794717D+00	1.147168775D-02	-2.220170412D-05				
1.995344981D-08	-6.090688740D-12		1.276501517D+04	1.461333093D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.650794328D+07	-7.711355860D+04	8.463771680D+01	-3.644250680D-02	8.403084420D-06				
-9.539882170D-10	4.264658030D-14		5.078931170D+05	-5.834656096D+02				

Mg2 Gurvich,1996a pt1 p393 pt2 p316.

2 tpis96 MG	2.00	0.00	0.00	0.00	0.00	0	48.6100000	286513.315
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.545195590D+03	4.115850040D+02	4.841196170D-01	4.891969650D-03	-6.395536840D-06				
4.299764550D-09	-1.164624418D-12		3.181641790D+04	2.640432143D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.038224994D+04	5.945240460D+01	2.352706666D+00	1.378537924D-04	-5.895692040D-08				
1.104045317D-11	-6.558868290D-16		3.351036560D+04	1.588177377D+01				

Mg2F4 Chase,1998 p1178.

2 j12/75 MG	2.00F	4.00	0.00	0.00	0.00	0	124.6036128	-1718369.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.511956137D+05	-3.122595912D+03	2.517715088D+01	-1.558723757D-02	1.552195619D-05				
-8.408729050D-09	1.911618525D-12		-1.953078883D+05	-1.085103537D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.980610166D+05	-1.201299868D+02	1.609110864D+01	-3.687456290D-05	8.220317050D-09				
-9.488869780D-13	4.419795330D-17		-2.117349690D+05	-5.308655470D+01				

## Appendix D (continued)

Mn Hf:Desai,1987. Sugar,1985. Gordon,1999.

3 g 7/97 MN	1.00	0.00	0.00	0.00	0.00	0	54.9380490	282400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.034061359D-01	-1.551537349D-03	2.500009148D+00	-2.723162066D-08	4.333897430D-11				
-3.511093890D-14	1.136032201D-17		3.321935190D+04	6.649325463D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.855155820D+03	8.838588440D+02	-3.648662580D-02	2.703720687D-03	-1.324971998D-06				
2.872603290D-10	-1.923633570D-14		2.867803487D+04	2.292541198D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.936189040D+09	-2.353549748D+06	5.377244800D+02	-5.824812570D-02	3.330475100D-06				
-9.689631050D-11	1.133286034D-15		1.879530161D+07	-4.690097890D+03				

Mn+ Sugar,1985. Gordon,1999.

3 g 6/97 MN	1.00E	-1.00	0.00	0.00	0.00	0	54.9375004	1005871.328
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.458017700D+02	-4.251151330D+00	2.521281028D+00	-5.565087280D-05	8.037162210D-08				
-6.093550970D-11	1.900014268D-14		1.202533602D+05	6.683468162D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.471314100D+05	-2.403796253D+03	5.937715750D+00	-2.341014594D-03	7.464165640D-07				
-9.075969730D-11	4.467879847D-15		1.349902108D+05	-1.702666341D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.717119921D+09	-9.029185830D+05	1.784788847D+02	-1.566770206D-02	7.346534410D-07				
-1.750673350D-11	1.667889239D-16		7.443546080D+06	-1.568005804D+03				

Mo Hf:Desai,1987. Sugar,1988. Gordon,1999.

3 g 7/97 MO	1.00	0.00	0.00	0.00	0.00	0	95.9400000	658500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.646367910D+01	-1.159269043D+00	2.506929462D+00	-2.099249725D-05	3.414779430D-08				
-2.841269591D-11	9.492443321D-15		7.845899800D+04	7.601835660D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.573271000D+06	-1.662365811D+04	2.135147077D+01	-1.003069377D-02	2.409784357D-06				
-1.811267352D-10	1.034189087D-15		1.842646473D+05	-1.275326434D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.205038910D+09	-3.855961600D+06	9.371595060D+02	-1.108164544D-01	6.929123900D-06				
-2.199865715D-10	2.798315513D-15		3.062163602D+07	-8.122811340D+03				

Mo+ Sugar,1988. Gordon,1999.

3 g 7/97 MO	1.00E	-1.00	0.00	0.00	0.00	0	95.9394514	1349012.928
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.298236623D+02	-1.560279908D+00	2.507600281D+00	-1.923789063D-05	2.673316651D-08				
-1.937174292D-11	5.729735412D-15		1.615103759D+05	7.442543460D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.298891120D+07	-3.948276230D+04	4.866599780D+01	-2.605352326D-02	7.215431920D-06				
-8.719164960D-10	3.788423040D-14		4.118948570D+05	-3.216791030D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.731253943D+09	8.776685240D+05	-1.669716753D+02	1.732439603D-02	-9.372726850D-07				
-2.593422324D-11	2.913787941D-16		-6.989098130D+06	1.517101780D+03				

Mo- Hotop,1985. Gordon,1999.

3 g10/97 MO	1.00E	1.00	0.00	0.00	0.00	0	95.9405486	580324.628
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		6.905123690D+04	7.485659540D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		6.905123690D+04	7.485659540D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		6.905123690D+04	7.485659540D+00				

MoO Gurvich,1982 pt1 p25 pt2 p30.

3 tps89 MO	1.000	1.00	0.00	0.00	0.00	0	111.9394000	358005.323
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.801152706D+04	5.139883480D+02	1.075385931D+00	8.681048470D-03	-1.11118984D-05				
7.234349330D-09	-1.893138381D-12		3.941374080D+04	2.272230239D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.573131992D+06	-5.241483580D+03	1.102656868D+01	-3.902996620D-03	1.147334134D-06				
-1.358975691D-10	5.775268580D-15		7.448972000D+04	-4.253612930D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.846838911D+08	-1.710122789D+05	4.036556200D+01	-2.750495204D-03	8.916821240D-08				
-1.248340135D-12	3.675821910D-18		1.408558917D+06	-3.171602770D+02				

## Appendix D (continued)

MoO2                      Gurvich,1982 pt1 p28 pt2 p33.

2 tpis82 MO	1.000	2.00	0.00	0.00	0.00	0.00	0	127.9388000	-15558.079
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.247183220D+04	-1.904783783D+02	2.120771647D+00	1.650280086D-02	-2.381696822D-05					
1.652371586D-08	-4.494452430D-12							-1.862932837D+03	1.640582056D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.096143654D+05	-1.932750274D+03	9.428673180D+00	-1.630508855D-03	5.752760170D-07					
-7.590457470D-11	3.461337780D-15							7.327725180D+03	-2.533315948D+01

MoO3                      Gurvich,1982 pt1 p31 pt2 p35.

2 tpis82 MO	1.000	3.00	0.00	0.00	0.00	0	143.9382000	-364412.371	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.977385360D+04	-7.684557830D+02	5.881844440D+00	1.686119817D-02	-2.582485043D-05					
1.850382718D-08	-5.152249850D-12							-4.155872390D+04	-6.529162160D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.097597270D+05	2.379066513D+02	9.311100800D+00	6.579338910D-04	-2.895307725D-07					
5.692637260D-11	3.489657310D-15							-4.923738720D+04	-2.114864892D+01

MoO3-                      Gurvich,1982 pt1 p32 pt2 p36.

2 tpis82 MO	1.000	3.00E	1.00	0.00	0.00	0	143.9387486	-655242.501	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.821617352D+05	-2.224656970D+03	1.320405967D+01	-1.249800352D-03	-1.864166983D-06					
2.276579470D-09	-7.366564570D-13							-6.938986000D+04	-4.699377210D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.881098720D+05	1.848536991D+01	1.042644941D+01	-6.265557910D-04	3.020554347D-07					
-4.733195890D-11	2.527517727D-15							-8.337815500D+04	-2.701522825D+01

Mo2O6                      Gurvich,1982 pt1 p33 pt2 p37.

2 tpis82 MO	2.000	6.00	0.00	0.00	0.00	0	287.8764000	-1149446.813	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.568375811D+05	-2.159930184D+03	1.522500503D+01	3.194198900D-02	-5.063877150D-05					
3.689371820D-08	-1.037872908D-11							-1.309931161D+05	-5.408918500D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.312238160D+05	-6.642827550D+02	2.249383570D+01	-1.968470329D-04	4.336740610D-08					
-4.959777990D-12	2.293212733D-16							-1.430573250D+05	-8.669628540D+01

Mo3O9                      Gurvich,1982 pt1 p34 pt2 p38.

2 tpis82 MO	3.000	9.00	0.00	0.00	0.00	0	431.8146000	-1902031.349	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.483386187D+05	-1.863895133D+03	1.738405871D+01	6.233012320D-02	-9.328441350D-05					
6.613638790D-08	-1.830607518D-11							-2.248945631D+05	-5.826669470D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.230290540D+05	-1.076171759D+03	3.480007260D+01	-3.189633800D-04	7.028397040D-08					
-8.039642640D-12	3.717879530D-16							-2.357422166D+05	-1.448769485D+02

Mo4O12                      Gurvich,1982 pt1 p36 pt2 p39.

2 tpis82 MO	4.000	12.00	0.00	0.00	0.00	0	575.7528000	-2625526.773	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.234876437D+05	-2.996203728D+03	2.682458827D+01	7.597345720D-02	-1.155247012D-04					
8.256472570D-08	-2.296764551D-11							-3.084619476D+05	-1.065236386D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.225283388D+06	-1.368141197D+03	4.701687810D+01	-4.052910200D-04	8.928472390D-08					
-1.021091158D-11	4.721091690D-16							-3.256477770D+05	-2.047486535D+02

Mo5O15                      Gurvich,1982 pt1 p38 pt2 p40.

2 tpis82 MO	5.000	15.00	0.00	0.00	0.00	0	719.6910000	-3329108.437	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.768903251D+05	-3.757933100D+03	3.408197760D+01	9.485414960D-02	-1.442672100D-04					
1.031163900D-07	-2.868600013D-11							-3.913507030D+05	-1.426449143D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.535389516D+06	-1.710367122D+03	5.927125780D+01	-5.066836290D-04	1.116223706D-07					
-1.276562233D-11	5.902318910D-16							-4.128972380D+05	-2.651287167D+02

N                          Hf:Cox,1989. Moore,1975. Gordon,1999.

3 g 5/97 N	1.00	0.00	0.00	0.00	0.00	0	14.0067000	472680.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00							5.610463780D+04	4.193905036D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.876501380D+04	-1.071231500D+02	2.362188287D+00	2.916720081D-04	-1.729515100D-07					
4.012657880D-11	-2.677227571D-15							5.697351330D+04	4.865231506D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.475181050D+08	-3.107574980D+05	6.916782740D+01	-6.847988130D-03	3.827572400D-07					
-1.098367709D-11	1.277986024D-16							2.550585618D+06	-5.848769753D+02



## Appendix D (continued)

N+ Moore,1975. Gordon,1999.

3 g 6/97 N	1.00E	-1.00	0.00	0.00	0.00	0	14.0061514	1882127.624
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.237079210D+03	2.299958315D+00	2.487488821D+00	2.737490756D-05	-3.134447576D-08				
1.850111332D-11	-4.447350984D-15		2.256284738D+05	5.076830786D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.904970374D+05	-8.557908610D+02	3.477389290D+00	-5.288267190D-04	1.352350307D-07				
-1.389834122D-11	5.046166279D-16		2.310809984D+05	-1.994146545D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.646092148D+07	-1.113165218D+04	4.976986640D+00	-2.005393583D-04	1.022481356D-08				
-2.691430863D-13	3.539931593D-18		3.136284696D+05	-1.706646380D+01				

N- Hotop,1985. Chase,1998 p1602. Gordon,1999.

3 j12/82 N	1.00E	1.00	0.00	0.00	0.00	0	14.0072486	473537.545
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.445682471D+03	7.335205110D+00	2.476680939D+00	4.227869180D-05	-4.426293320D-08				
2.490985431D-11	-5.831608090D-15		5.617625000D+04	5.145753977D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.404189576D+03	2.954965336D-01	2.499789368D+00	8.307564970D-08	-1.829942770D-11				
2.100136461D-15	-9.754986710D-20		5.621413890D+04	5.006484157D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.884379470D+03	3.905516910D-01	2.499914043D+00	9.818512540D-09	-6.126037340D-13				
1.980010689D-17	-2.593295116D-22		5.621304520D+04	5.005647607D+00				

NCO Hf:East,1993. Jacox,1998 p184.

2 g 6/01 N	1.00C	1.00	0.00	0.00	0.00	0	42.0168000	131847.241
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.136503036D+04	-2.444613367D+02	4.671376100D+00	2.309387548D-03	2.798649599D-06				
-4.546357380D-09	1.692880931D-12		1.577649188D+04	-2.171476903D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.089445289D+05	-1.735459316D+03	8.655610330D+00	-4.053229260D-04	7.599716410D-08				
-7.253804150D-12	3.244872410D-16		2.365792776D+04	-2.619532970D+01				

ND Hf:est. from NH,H&D data. Chase,1998 p1037 6/77.

2 g 4/01 N	1.00D	1.00	0.00	0.00	0.00	0	16.0208020	355738.797
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.290155757D+04	-3.957388510D+02	6.179010330D+00	-8.847806970D-03	1.441582970D-05				
-1.006647227D-08	2.654403586D-12		4.355913430D+04	-1.180414072D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.439657960D+05	-2.084583507D+03	5.834089720D+00	-4.189393360D-04	9.768929530D-08				
-1.056317654D-11	4.683079210D-16		5.466633410D+04	-1.480810939D+01				

ND2 Hf:est. from NH2,H,&D data. Jacox,1998 p133.

2 g 4/01 N	1.00D	2.00	0.00	0.00	0.00	0	18.0349040	184836.570
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.935222164D+04	-2.130631713D+02	4.844017600D+00	-2.516949288D-03	7.616381540D-06				
-5.464501770D-09	1.292736999D-12		2.211998374D+04	-3.171712417D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.631308357D+06	-6.564637490D+03	1.280547961D+01	-3.094456779D-03	9.181660230D-07				
-1.241119284D-10	6.226299860D-15		6.108929580D+04	-6.124502693D+01				

ND3 Hf:est. from NH3,H,&D data. Chase,1998 p1047 6/77.

2 g 4/01 N	1.00D	3.00	0.00	0.00	0.00	0	20.0490060	-54752.106
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.045120370D+04	1.610166943D+02	8.574963230D-01	1.319688794D-02	-1.153090144D-05				
7.142495560D-09	-2.109194351D-12		-8.220948900D+03	1.675921299D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.599516958D+06	-1.013420124D+04	1.798028169D+01	-3.582609800D-03	1.009922000D-06				
-1.537638609D-10	9.106175650D-15		5.397205660D+04	-9.810988569D+01				

NF Gurvich,1989 pt1 p372 pt2 p234. Gurvich,1978 pt2 p243.

2 tps189 N	1.00F	1.00	0.00	0.00	0.00	0	33.0051032	232990.500
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.504927750D+04	6.674502990D+02	-1.201665982D+00	1.452074253D-02	-1.822873148D-05				
1.160136864D-08	-2.973416333D-12		2.395414002D+04	3.089260431D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.002987330D+05	-3.237696580D+03	8.703408870D+00	-2.701025798D-03	9.150042110D-07				
-1.365256630D-10	7.234624410D-15		4.642819450D+04	-3.019933248D+01				

NF2 Gurvich,1989 pt1 p373. McBride,1992 METHOD NRRAO1.

2 g 4/99 N	1.00F	2.00	0.00	0.00	0.00	0	52.0035064	34421.447
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.511831104D+04	9.196389940D+01	4.947301790D-01	2.001847323D-02	-2.767712684D-05				
1.872924867D-08	-5.020318040D-12		2.839279606D+03	2.270515670D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.945010078D+05	-3.536034070D+02	7.263494360D+00	-8.402380400D-05	2.326721111D-08				
-2.667577562D-12	1.236070614D-16		3.435440590D+03	-1.336102511D+01				

## Appendix D (continued)

NF3                      Gurvich,1989 pt1 p375. McBride,1992 METHOD NRRAO2.

2 g 4/99 N	1.00F	3.00	0.00	0.00	0.00	0.00	0	71.0019096	-131700.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.757149280D+04	-9.031832890D+02	4.027417270D+00	2.314439555D-02	-3.415106470D-05					
2.409483651D-08	-6.633464190D-12							-1.237232074D+04	3.026430713D-01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.496268760D+05	-4.973728670D+02	1.036866128D+01	8.900687650D-05	5.882654360D-08					
-3.157737664D-12	1.714329953D-16							-1.713183352D+04	-3.098920858D+01

NH                      Hf:Anderson,1989. Gurvich,1978 pt2 p223.

3 g 4/99 N	1.00H	1.00	0.00	0.00	0.00	0	15.0146400	357032.001	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.359651320D+04	-1.900296604D+02	4.518496790D+00	-2.432776899D-03	2.377587464D-06					
-2.592797084D-10	-2.659680792D-13							4.280972190D+04	-3.886561616D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.958141991D+06	-5.782861300D+03	9.335742020D+00	-2.292910311D-03	6.076092480D-07					
-6.647942190D-09	2.384234783D-15							7.898912340D+04	-4.116970400D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.524636790D+07	-8.585826910D+04	2.980445181D+01	-2.979563697D-03	1.656334158D-07					
-4.744791840D-12	5.570148290D-17							6.961434270D+05	-2.229027419D+02

NH+                      Hf:Gibson,1985. Gurvich,1989 pt2 p216.

3 g 5/99 N	1.00H	1.00E	-1.00	0.00	0.00	0	15.0140914	1665787.914	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.253656850D+03	-2.458222206D+02	6.708919490D+00	-1.038489430D-02	1.509008623D-05					
-9.580512190D-09	2.333206758D-12							2.001077797D+05	-1.395057632D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.405709438D+06	-4.136215710D+03	7.632014480D+00	-1.228325778D-03	2.721187746D-07					
-2.010098289D-11	3.717190180D-17							2.258975960D+05	-2.786785234D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.392941759D+08	-1.741658624D+05	5.107907910D+01	-5.567623700D-03	3.273391600D-07					
-9.797978060D-12	1.186543279D-16							1.554705305D+06	-4.065968960D+02

NHF                      Gurvich,1989 pt1 p386 pt2 p247.

2 tpis89 N	1.00H	1.00F	1.00	0.00	0.00	0	34.0130432	112000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.110659820D+04	9.612256430D+02	-2.706446594D+00	2.036562680D-02	-2.425558952D-05					
1.551553017D-08	-4.058458260D-12							7.909628340D+03	4.099317124D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.013902720D+05	-3.463397050D+03	8.705804860D+00	-4.018963410D-04	2.322774501D-08					
6.280487330D-12	-6.283095690D-16							3.337065340D+04	-2.900483634D+01

NHF2                      Gurvich,1989 pt1 p388 pt2 p249.

2 tpis89 N	1.00H	1.00F	2.00	0.00	0.00	0	53.0114464	-103000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.626113420D+04	1.205756556D+03	-6.017529420D+00	3.760027690D-02	-4.619198600D-05					
2.942475570D-08	-7.598732360D-12							-1.897014374D+04	5.901714907D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.394278990D+05	-4.004471770D+03	1.221322320D+01	-6.970437730D-04	1.271073981D-07					
-1.247136898D-11	5.086517590D-16							9.134195980D+03	-4.867843963D+01

NH2                      Hf:Anderson,1989. Gurvich,1989 pt1 p349. Jacox,1998 p133.

2 g 3/01 N	1.00H	2.00	0.00	0.00	0.00	0	16.0225800	189134.713	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.118240659D+04	4.754243390D+02	1.372395176D+00	6.306429720D-03	-5.987893560D-06					
4.492752340D-09	-1.414073548D-12							1.928939662D+04	1.540126885D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.111053740D+06	-6.880627230D+03	1.132305924D+01	-1.829236741D-03	5.643890090D-07					
-7.886452480D-11	4.078593450D-15							6.503778560D+04	-5.359155744D+01

NH2F                      Gurvich,1989 pt1 p387 pt2 p248.

2 tpis89 N	1.00H	2.00F	1.00	0.00	0.00	0	35.0209832	-75000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.092374760D+05	1.844919780D+03	-7.673871600D+00	3.229533440D-02	-3.388108670D-05					
1.971871550D-08	-4.810205150D-12							-1.878318960D+04	6.861483739D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.927205340D+06	-7.500447160D+03	1.395589580D+01	-1.184804420D-03	2.050678670D-07					
-1.908761310D-11	7.389236210D-16							3.552927340D+04	-6.731185491D+01

NH3                      Gurvich,1989 pt1 p354 pt2 p219. Haar,1968.

2 tpis89 N	1.00H	3.00	0.00	0.00	0.00	0	17.0305200	-45940.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.681226150D+04	1.270951578D+03	-3.893229130D+00	2.145988418D-02	-2.183766703D-05					
1.317385706D-08	-3.332322060D-12							-1.264886413D+04	4.366014588D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.452389535D+06	-8.040894240D+03	1.271346201D+01	-3.980186580D-04	3.552502750D-08					
2.530923570D-12	-3.322700530D-16							4.386191960D+04	-6.462330602D+01

## Appendix D (continued)

NH<sub>2</sub>OH                      Hydroxylamine. Gurvich,1989 pt1 p368 pt2 p232.

2 tpi89 N	1.00H	3.000	1.00	0.00	0.00	0	33.0299200	-50000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								11235.778

-5.617586670D+04 1.209290057D+03-6.179599060D+00 4.053116440D-02-5.190105540D-05  
3.594544580D-08-9.933681640D-12 -1.265888352D+04 5.727932928D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11235.778  
4.878285050D+06-1.533604636D+04 2.227239990D+01-2.514583678D-03 3.339589730D-07  
-1.881744532D-11 1.918174365D-16 8.923020710D+04-1.269053624D+02

NH<sub>4</sub><sup>+</sup>                      Gurvich,1989 pt1 p355 pt2 p220.

2 tpi89 N	1.00H	4.00E	-1.00	0.00	0.00	0	18.0379114	644904.945
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								9978.772

-2.668315752D+05 3.763020690D+03-1.571327725D+01 4.548820210D-02-4.379962120D-05  
2.464478293D-08-5.961532330D-12 5.823284720D+04 1.112087156D+02  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9978.772  
4.141889000D+06-1.442072042D+04 2.011893564D+01-1.971492619D-03 3.112721421D-07  
-2.602979969D-11 8.894342130D-16 1.664196236D+05-1.201535761D+02

NO                      Gurvich,1978,1989 pt1 p326 pt2 p203.

3 tpi89 N	1.000	1.00	0.00	0.00	0.00	0	30.0061000	91271.310
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								9179.110

-1.143916503D+04 1.536467592D+02 3.431468730D+00-2.668592368D-03 8.481399120D-06  
-7.685111050D-09 2.386797655D-12 9.098214410D+03 6.728725490D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9179.110  
2.239018716D+05-1.289651623D+03 5.433936030D+00-3.656034900D-04 9.880966450D-08  
-1.416076856D-11 9.380184620D-16 1.750317656D+04-8.501669090D+00  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9179.110  
-9.575303540D+08 5.912434480D+05-1.384566826D+02 1.694339403D-02-1.007351096D-06  
-2.912584076D-11-3.295109350D-16 -4.677501240D+06 1.242081216D+03

NO<sub>2</sub>                      Cp,S,IP(NO): Gurvich,1989 pt1 p330 pt2 p205.

3 g 5/99 N	1.000	1.00E	-1.00	0.00	0.00	0	30.0055514	990809.704
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								8670.104

1.398106635D+03-1.590446941D+02 5.122895400D+00-6.394388620D-03 1.123918342D-05  
-7.988581260D-09 2.107383677D-12 1.187495132D+05-4.398433810D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8670.104  
6.069876900D+05-2.278395427D+03 6.080324670D+00-6.066847580D-04 1.432002611D-07  
-1.747990522D-11 8.935014060D-16 1.322709615D+05-1.519880037D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8670.104  
2.676400347D+09-1.832948690D+06 5.099249390D+02-7.113819280D-02 5.317659880D-06  
-1.963208212D-10 2.805268230D-15 1.443308939D+07-4.324044462D+03

NOCL                      Gurvich,1989 pt1 p389. McBride,1992 METHOD PANDK.

2 g 4/99 N	1.000	1.00CL	1.00	0.00	0.00	0	65.4591000	52698.828
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								11364.488

2.308835209D+04-5.495983840D+02 7.730463360D+00-5.073910900D-03 1.062996184D-05  
-8.793249700D-09 2.648180166D-12 7.389898390D+03-1.318393021D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11364.488  
-6.133413330D+05-3.919298830D+02 9.138917220D+00-2.605664613D-03 1.295687247D-06  
-2.215378352D-10 1.280394898D-14 4.517328420D+03-2.307323335D+01

NOF                      Gurvich,1989 pt1 p382. McBride,1992 METHOD NRRAO2.

2 g 4/99 N	1.000	1.00F	1.00	0.00	0.00	0	49.0045032	-65000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								10720.271

4.755024260D+04-7.253904170D+02 7.213996360D+00-2.532427181D-03 6.377743900D-06  
-5.518305880D-09 1.681935713D-12 -5.609722520D+03-1.289663616D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10720.271  
1.889069274D+06-6.731022660D+03 1.419018767D+01-3.693124620D-03 9.938575140D-07  
-1.080748188D-10 4.210354430D-15 3.209900780D+04-6.370266962D+01

NOF<sub>3</sub>                      Gurvich,1989 pt1 p385 pt2 p246.

2 tpi89 N	1.000	1.00F	3.00	0.00	0.00	0	87.0013096	-187000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								13697.653

1.488360135D+05-2.241049812D+03 1.302355027D+01 5.463976680D-03-8.641865250D-06  
5.913659030D-09-1.577009169D-12 -1.328342568D+04-4.877320739D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13697.653  
-2.785625217D+05-1.252321663D+03 1.390824337D+01-3.566687500D-04 7.785011060D-08  
-8.850411970D-12 4.075980030D-16 -2.025651446D+04-5.106881859D+01

NO<sub>2</sub>                      Gurvich,1989 pt1 p332 pt2 p207.

2 g 4/99 N	1.000	2.00	0.00	0.00	0.00	0	46.0055000	34193.019
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
								10208.175

-5.642038780D+04 9.633085720D+02-2.434510974D+00 1.927760886D-02-1.874559328D-05  
9.145497730D-09-1.777647635D-12 -1.547925037D+03 4.067851210D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10208.175  
7.213001570D+05-3.832615200D+03 1.113963285D+01-2.238062246D-03 6.547723430D-07  
-7.611335900D-11 3.328361050D-15 2.502497403D+04-4.305130040D+01

## Appendix D (continued)

NO2- Gurvich,1989 pt1 p334 pt2 p208.

2 tpis89 N	1.000	2.00E	1.00	0.00	0.00	0	46.0060486	-200035.591
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10177.009

-1.282067858D+04 6.990138180D+02-2.812596273D+00 2.412894252D-02-2.831606689D-05  
1.670509365D-08-3.983330130D-12 -2.809915579D+04 4.063271510D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10177.009  
1.325710335D+05-1.557032129D+03 8.126721920D+00-2.728626780D-04-4.707541800D-08  
2.826729008D-11-2.353985481D-15 -1.715795217D+04-2.228576043D+01

NO2CL Gurvich,1989 pt1 p391. McBride,1992 METHOD NRRAO1.

2 g 4/99 N	1.000	2.00CL	1.00	0.00	0.00	0	81.4585000	12500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								12204.839

8.508370340D+03-1.805383762D+02 3.785388560D+00 1.414934934D-02-1.423946765D-05  
7.028226180D-09-1.374688214D-12 9.156246470D+02 6.958904458D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12204.839  
-1.086773327D+05-1.452231167D+03 1.105656962D+01-4.000099280D-04 9.101543040D-08  
-1.036656913D-11 4.781664810D-16 6.294267320D+03-3.521239681D+01

NO2F Gurvich,1989 pt1 p349. McBride,1992 METHOD NRRAO1.

2 g 4/99 N	1.000	2.00F	1.00	0.00	0.00	0	65.0039032	-109000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								11346.581

5.667856950D+04-6.538251950D+02 4.472771520D+00 1.368870672D-02-1.460533236D-05  
7.779227940D-09-1.689355106D-12 -1.102179443D+04 3.292074310D-01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11346.581  
-1.008577842D+05-1.704722752D+03 1.122954945D+01-4.685215970D-04 1.047692566D-07  
-1.189150595D-11 5.470307120D-16 -6.891719180D+03-3.849788492D+01

NO3 Chase,1998 p1607.

2 j12/64 N	1.000	3.00	0.00	0.00	0.00	0	62.0049000	71128.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10958.914

3.405398410D+04 2.266670652D+02-3.793081630D+00 4.170732700D-02-5.709913270D-05  
3.834158110D-08-1.021969284D-11 7.088112200D+03 4.273091713D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10958.914  
-3.943872710D+05-8.244263530D+02 1.061325843D+01-2.448749816D-04 5.406060320D-08  
-6.195466750D-12 2.870000149D-16 8.982011730D+03-3.444666597D+01

NO3- Gurvich,1989 pt1 p335 pt2 p209.

2 tpis89 N	1.000	3.00E	1.00	0.00	0.00	0	62.0054486	-310779.531
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								10773.105

9.204813610D+04-3.911171150D+02-2.354356764D-01 2.836042108D-02-3.461324080D-05  
2.081787460D-08-5.021601270D-12 -3.576411500D+04 2.299942308D+01  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10773.105  
-3.110005758D+05-1.369087552D+03 1.101342913D+01-4.036878820D-04 8.902086470D-08  
-1.019733480D-11 4.723330790D-16 -3.364321090D+04-3.878432657D+01

NO3F Gurvich,1989 pt1 p384 pt2 p245.

2 tpis89 N	1.000	3.00F	1.00	0.00	0.00	0	81.0033032	15000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								14444.156

6.472832030D+04-8.213134310D+02 6.194917440D+00 1.805438628D-02-1.996693240D-05  
1.124482018D-08-2.680013077D-12 4.206661790D+03-7.016104301D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14444.156  
-3.411793300D+05-2.353908798D+03 1.628114887D+01-1.910415273D-03 4.690873560D-07  
-5.686040140D-11 2.720906921D-15 9.760583980D+03-6.558153684D+01

N2 Ref-Elm. Gurvich,1978 pt1 p280 pt2 p207.

3 tpis78 N	2.00	0.00	0.00	0.00	0.00	0	28.0134000	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+02-1.076003744D+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+04-1.586640027D+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+06-1.672099740D+03

N2+ Gurvich,1989 pt1 p323 pt2 p200.

3 tpis89 N	2.00E	-1.00	0.00	0.00	0.00	0	28.0128514	1509508.424
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8671.100

-3.474047470D+04 2.696222703D+02 3.164916370D+00-2.132239781D-03 6.730476400D-06  
-5.637304970D-09 1.621756000D-12 1.790004424D+05 6.832974166D+00  
1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8671.100  
-2.845599002D+06 7.058893030D+03-2.884886385D+00 3.068677059D-03-4.361652310D-07  
2.102514545D-11 5.411996470D-16 1.340388483D+05 5.090897022D+01  
6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8671.100  
-3.712829770D+08 3.139287234D+05-9.603518050D+01 1.571193286D-02-1.175065525D-06  
4.144441230D-11-5.621893090D-16 -2.217361867D+06 8.436270947D+02

## Appendix D (continued)

N2- Chase,1998 p1623.

3 j 9/77 N	2.00E	1.00	0.00	0.00	0.00	0.00	0.00	28.0139486	148183.282
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.146227110D+04	9.063600790D+02	-1.520054079D-01	6.023190840D-03	-2.897138445D-06					
-4.129106680D-11	3.206989770D-13		1.218808548D+04	2.638068855D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									8674.282
2.169637706D+05	-1.275098516D+03	5.391095700D+00	-3.198907510D-04	7.311051350D-08					
-8.202017370D-12	3.740044700D-16		2.424964308D+04	-9.014934294D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									8674.282
1.345850786D+06	-1.060565497D+03	4.732026850D+00	-5.091450050D-06	1.628212099D-09					
-5.224243560D-14	6.796651250D-19		2.394627677D+04	-4.297861544D+00					

NCN Hf:Gurvich,1991 pt1 p219. Jacox,1998 p180.

2 g 6/01 N	2.00C	1.00	0.00	0.00	0.00	0.00	0.00	40.0241000	500456.573
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									10180.177
-5.634680700D+04	7.323804580D+02	-7.821401840D-01	1.838552441D-02	-1.950836491D-05					
1.035712021D-08	-2.208158483D-12		5.539789700D+04	2.905308985D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									10180.177
-1.641880975D+05	-7.767840750D+02	7.999981870D+00	-1.659081508D-04	2.983403318D-08					
-3.120157047D-12	1.992698720D-16		6.184424480D+04	-2.149108820D+01					

N2D2,cis Hf:Use NASA data for N2H2,H,&D. Chase,1998 p1044 6/77.

2 g 6/01 N	2.00D	2.00	0.00	0.00	0.00	0.00	0.00	32.0416040	202857.330
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									10308.037
-2.743733656D+04	7.149808830D+02	-2.223247620D+00	2.088722282D-02	-1.821711897D-05					
8.844079940D-09	-1.918010649D-12		2.011115649D+04	3.637100195D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									10308.037
8.798074710D+05	-5.299362040D+03	1.355007485D+01	-1.316635227D-03	2.755816197D-07					
-3.036294387D-11	1.365324117D-15		5.356311890D+04	-6.271215875D+01					

N2F2 Gurvich,1989 pt1 p377 pt2 p237.

2 tpis89 N	2.00F	2.00	0.00	0.00	0.00	0.00	0.00	66.0102064	62373.546
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									12868.756
1.543893150D+04	-2.183635130D+02	3.890284250D+00	1.674017740D-02	-2.056393090D-05					
1.258692110D-08	-3.110498290D-12		7.052038700D+03	5.265866442D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									12868.756
-1.824883860D+05	-9.534029960D+02	1.069795480D+01	-2.759968700D-04	6.055439700D-08					
-6.911215080D-12	3.192587230D-16		9.283466960D+03	-3.246968772D+01					

N2F4 Gurvich,1989 pt1 p380 pt2 p240.

2 tpis89 N	2.00F	4.00	0.00	0.00	0.00	0.00	0.00	104.0070128	-22000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									17811.571
1.162914512D+05	-1.538660418D+03	9.054033050D+00	2.862113563D-02	-4.332286990D-05					
3.067642499D-08	-8.455474110D-12		2.865277526D+03	-2.476493006D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									17811.571
-5.188594710D+05	-6.702256510D+02	1.650109262D+01	-2.006404436D-04	4.436752510D-08					
-5.089808880D-12	2.359374159D-16		-5.281488900D+03	-6.040513435D+01					

N2H2 Gurvich,1989 pt1 p356.Trans,cis,& 1,1 in equilibrium.

2 g 5/99 N	2.00H	2.00	0.00	0.00	0.00	0.00	0.00	30.0292800	211858.756
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									9996.961
-1.504005163D+05	2.346687716D+03	-9.405430290D+00	3.284299800D-02	-3.121920401D-05					
1.721283190D-08	-4.014537220D-12		1.319384041D+04	7.832382630D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									9996.961
6.217567870D+06	-1.753952096D+04	2.022730509D+01	-9.757297660D-04	-4.208416740D-07					
1.117921171D-10	-7.627102210D-15		1.374152574D+05	-1.199559168D+02					

NH2NO2 Aminyl Nitrite. Gurvich,1989 pt1 p370 pt2 p233.

2 tpis89 N	2.00H	2.00	0.00	0.00	0.00	0.00	0.00	62.0280800	-26000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									12163.853
-4.573035060D+04	1.201365987D+03	-8.105984110D+00	5.402715200D-02	-6.438074450D-05					
4.025097920D-08	-1.025154190D-11		-9.615785160D+03	6.867353357D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									12163.853
1.654040575D+06	-8.125220880D+03	2.021742772D+01	-1.244291821D-03	2.122804183D-07					
-1.948359653D-11	7.439351360D-16		4.230822580D+04	-1.016190179D+02					

N2H4 Gurvich,1989 pt1 p360 pt2 p225.

2 g 4/99 N	2.00H	4.00	0.00	0.00	0.00	0.00	0.00	32.0451600	95180.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									11449.304
-1.660756354D+05	3.035416736D+03	-1.736889823D+01	7.159834020D-02	-8.866799300D-05					
5.798970280D-08	-1.530037218D-11		-3.731927230D+03	1.190002218D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
									11449.304
3.293486700D+06	-1.199850628D+04	2.104406814D+01	-1.399381724D-03	1.933173351D-07					
-1.318016127D-11	3.166400170D-16		8.348433700D+04	-1.155751024D+02					

## Appendix D (continued)

N2O Gurvich,1989 pt1 p337 pt2 p210.

2 g 4/99 N	2.000	1.00	0.00	0.00	0.00	0.00	0	44.0128000	81600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.288225970D+04	-6.440118440D+02	6.034351430D+00	2.265394436D-04	3.472782850D-06					
-3.627748640D-09	1.137969552D-12		1.179405506D+04	-1.003128570D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.438448040D+05	-2.404557558D+03	9.125636220D+00	-5.401667930D-04	1.315124031D-07					
-1.414215100D-11	6.381066870D-16		2.198632638D+04	-3.147805016D+01					

N2O+ Chase,1998 p1625.

2 j12/70 N	2.000	1.00E	-1.00	0.00	0.00	0	44.0122514	1332956.507	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.624147080D+04	6.696211610D+02	8.781456190D-02	1.524476027D-02	-1.527290811D-05					
7.827237390D-09	-1.646739623D-12		1.557295192D+05	2.562354785D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.983553254D+04	-1.179455967D+03	8.300186690D+00	-2.887267217D-04	5.705105010D-08					
-5.958885120D-12	2.835725557D-16		1.646021769D+05	-2.287356617D+01					

N2O3 Gurvich,1989 pt1 p338 pt2 p211.

2 g 4/99 N	2.000	3.00	0.00	0.00	0.00	0	76.0116000	86630.595	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.204444170D+04	9.295520150D+02	3.203664810D+00	1.356473078D-02	-6.262966070D-06					
-1.402915559D-09	1.431620930D-12		3.313622080D+03	1.844430953D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.783881860D+05	-4.483024660D+03	1.666668024D+01	-2.062143878D-03	5.309541710D-07					
-6.190451220D-11	2.692956658D-15		3.360912450D+04	-6.739212388D+01					

N2O4 Gurvich,1989 pt1 p342 pt2 p212.

2 tpis89 N	2.000	4.00	0.00	0.00	0.00	0	92.0110000	11110.919	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.804751440D+04	5.612828890D+02	-2.083648324D-01	3.887087820D-02	-4.422412260D-05					
2.498812310D-08	-5.679102380D-12		-3.310794730D+03	2.963924840D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.582843760D+05	-1.604749805D+03	1.674102133D+01	-5.091385080D-04	1.143634670D-07					
-1.316288176D-11	5.976316620D-16		4.306900520D+03	-6.569450380D+01					

N2O5 Gurvich,1989 pt1 p343 pt2 p213.

2 g 4/99 N	2.000	5.00	0.00	0.00	0.00	0	108.0104000	13300.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.007828170D+04	-8.769675120D+02	1.055932981D+01	1.394613859D-02	-8.884346920D-06					
8.500431150D-10	7.791550910D-13		3.038962037D+03	-2.386831860D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.325578960D+04	-3.109277389D+03	2.036088958D+01	-9.959901140D-04	2.401398635D-07					
-3.057161911D-11	1.495915511D-15		1.336957281D+04	-8.298623341D+01					

N3 Gurvich,1989 pt1 p325 pt2 p202.

2 tpis89 N	3.00	0.00	0.00	0.00	0.00	0	42.0201000	436000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.337406790D+04	-2.965683604D+02	3.314279150D+00	6.721685360D-03	-4.181126390D-06					
8.618442360D-10	6.883352530D-14		5.298840620D+04	5.312776486D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.529264658D+05	-2.362876591D+03	9.135267130D+00	-6.212870850D-04	1.324094351D-07					
-1.478989640D-11	6.721230470D-16		6.412695390D+04	-3.135825973D+01					

N3H Gurvich,1989 pt1 p362 pt2 p226.

2 g 4/99 N	3.00H	1.00	0.00	0.00	0.00	0	43.0280400	294000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.242576060D+03	6.692664890D+01	1.766142217D+00	1.487411419D-02	-1.539086440D-05					
9.172303550D-09	-2.337205474D-12		3.392069700D+04	1.513752057D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.170469241D+06	-5.102451990D+03	1.278288910D+01	-8.409487160D-04	1.592142834D-07					
-1.512289051D-11	6.102906630D-16		6.428344470D+04	-5.513119108D+01					

Na Hf:Cox,1989. Martin,1981. Gordon,1999.

3 g 8/97 NA	1.00	0.00	0.00	0.00	0.00	0	22.9897700	107500.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		1.218382949D+04	4.244028180D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.525723380D+05	-2.623807254D+03	5.162596620D+00	-1.210218586D-03	2.306301844D-07					
-1.249597843D-11	7.226771190D-16		2.912963564D+04	-1.519717061D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.592533392D+09	-9.717836660D+05	2.238443963D+02	-2.380930558D-02	1.352018117D-06					
-3.936971110D-11	4.630689121D-16		7.748677260D+06	-1.939615505D+03					

## Appendix D (continued)

Na+ Martin,1981. Gordon,1999.

3 g 1/98 NA	1.00E	-1.00	0.00	0.00	0.00	0	22.9892214	609542.928
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						7.256537070D+04	3.550845080D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						7.256537070D+04	3.550845080D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.401202990D+04	-2.137774622D+01	2.505443851D+00	-7.186631690D-07	5.188796390D-11				
-1.944511626D-15	2.959355125D-20		7.273413620D+04	3.503904060D+00				

Na- Hotop,1985. Gordon,1999.

3 g 4/97 NA	1.00E	1.00	0.00	0.00	0.00	0	22.9903186	48453.428
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000001D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						5.082199670D+03	3.550916790D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000001D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						5.082199670D+03	3.550916790D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000001D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						5.082199670D+03	3.550916790D+00

NaAlF4 Gurvich,1982 pt1 p359 pt2 p393.

2 tpis82 NA	1.00AL	1.00F	4.00	0.00	0.00	0	125.9649208	-1857841.546
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.315359536D+05	-2.394685695D+03	1.909539612D+01	1.044339733D-03	-6.949754130D-06				
6.769098140D-09	-2.176199098D-12		-2.150512366D+05	-7.505102130D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.571177930D+05	-2.496543879D+02	1.618634511D+01	-7.449049300D-05	1.644510872D-08				
-1.883696066D-12	8.719877450D-17		-2.279533538D+05	-5.370665140D+01				

NaBO2 Gurvich,1982 pt1 p358 pt2 p392.

2 tpis82 NA	1.00B	1.00O	2.00	0.00	0.00	0	65.7995700	-633449.330
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.046867360D+04	-8.699970600D+02	8.942208240D+00	1.092655824D-03	1.440608828D-06				
-2.254633535D-09	8.123312850D-13		-7.378318360D+04	-1.951815135D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.595814050D+04	-1.691902222D+03	1.118847517D+01	-4.564202310D-04	9.804505160D-08				
-1.101655008D-11	5.029172760D-16		-6.949292060D+04	-3.416353130D+01				

NaBr Gurvich,1982 pt1 p342 pt2 p379.

2 tpis82 NA	1.00BR	1.00	0.00	0.00	0.00	0	102.8937700	-145928.882
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.466827136D+04	7.622282870D+01	3.921163470D+00	1.793780908D-03	-2.457391648D-06				
1.739334522D-09	-4.796701380D-13		-1.926491755D+04	6.404382860D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.978513020D+05	-2.697899721D+03	7.545377160D+00	-1.566692184D-03	4.470392740D-07				
-4.832810210D-11	1.423961300D-15		-1.750862247D+03	-1.856478949D+01				

NaCN Chase,1998 p634.

2 j 3/66 NA	1.00C	1.00N	1.00	0.00	0.00	0	49.0071700	94266.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.446165410D+04	-7.536019970D+02	1.044966241D+01	-1.168769048D-02	1.849279385D-05				
-1.319387974D-08	3.589766560D-12		1.297820493D+04	-2.988519681D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.665570290D+05	-1.782094358D+03	8.699622630D+00	-4.463297000D-04	9.362229310D-08				
-1.033071320D-11	4.650466810D-16		2.010926347D+04	-2.419276094D+01				

NaCl Gurvich,1982 pt1 p337 pt2 p375.

2 tpis82 NA	1.00CL	1.00	0.00	0.00	0.00	0	58.4427700	-181544.884
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.362378350D+04	-7.583034460D+02	8.259173000D+00	-9.640915140D-03	1.358854616D-05				
-9.667032250D-09	2.746261290D-12		-1.950409477D+04	-1.936687551D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.314498760D+05	-8.968315650D+02	5.277287380D+00	-1.475674008D-04	-1.491128988D-08				
2.465673596D-11	-2.730355213D-15		-1.736277667D+04	-3.998288560D+00				

NaF Gurvich,1982 pt1 p332 pt2 p371.

2 tpis82 NA	1.00F	1.00	0.00	0.00	0.00	0	41.9881732	-295156.889
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.959887440D+04	-6.534626070D+02	6.941173200D+00	-5.307814930D-03	6.979720660D-06				
-4.820425730D-09	1.364849175D-12		-3.352940890D+04	-1.403212229D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.092926912D+06	3.293303640D+03	4.135919840D-01	2.634994470D-03	-8.384295630D-07				
1.417053025D-10	-8.600270160D-15		-5.772884630D+04	2.909489906D+01				

## Appendix D (continued)

NaH Gurvich,1982 pt1 p326 pt2 p366.

2 tps82 NA	1.00H	1.00	0.00	0.00	0.00	0.00	0	23.9977100	140835.105
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.222206410D+04	6.237622010D+02	-9.216277510D-01	1.360765851D-02	-1.659249878D-05					
1.033284544D-08	-2.589726392D-12		1.307381654D+04	2.641418597D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.756184750D+06	1.452047626D+04	-1.327563485D+01	1.055828277D-02	-2.990041189D-06					
3.905322880D-10	-1.923931194D-14		-7.632922270D+04	1.222070060D+02					

NaI Gurvich,1982 pt1 p345 pt2 p382.

2 tps82 NA	1.00I	1.00	0.00	0.00	0.00	0	149.8942400	-90637.880
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.228868506D+04	-2.857192800D+02	5.961057000D+00	-3.792532580D-03	5.566881310D-06				
-4.045013680D-09	1.172998933D-12		-1.088250556D+04	-3.990739920D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.281549408D+06	-7.093156630D+03	1.304994968D+01	-5.013492330D-03	1.581735155D-06				
-2.285837754D-10	1.195889950D-14		3.253893620D+04	-5.640023320D+01				

NaLi Gurvich,1982 pt1 p363 pt2 p396.

2 tps82 NA	1.00LI	1.00	0.00	0.00	0.00	0	29.9307700	178598.320
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.569992760D+03	-5.253940430D+00	4.329384260D+00	1.097919189D-03	-1.965726597D-06				
2.086472026D-09	-8.195988110D-13		2.016224293D+04	1.413253322D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.091664860D+07	-3.480010640D+04	4.614311920D+01	-2.260951051D-02	5.685324370D-06				
-6.458143300D-10	2.696508992D-14		2.394431755D+05	-2.961780126D+02				

NaNO2 Gurvich,1982 pt1 p352 pt2 p387.

2 g10/99 NA	1.00N	1.000	2.00	0.00	0.00	0	68.9952700	-166292.779
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.934460610D+04	1.115432670D+03	-1.816284973D+00	2.916366016D-02	-3.505788520D-05				
2.128602855D-08	-5.226211990D-12		-2.707275053D+04	4.121853253D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.765557495D+05	-8.635212950D+02	1.064105940D+01	-2.559465044D-04	5.654465630D-08				
-6.486710320D-12	3.008171243D-16		-1.868435672D+04	-2.921304474D+01				

NaNO3 Gurvich,1982 pt1 p355 pt2 p389.

2 tps82 NA	1.00N	1.000	3.00	0.00	0.00	0	84.9946700	-285528.711
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.043852507D+04	6.917093410D+02	-2.397485012D+00	4.100386430D-02	-5.141702580D-05				
3.228622470D-08	-8.164691600D-12		-3.906401320D+04	4.174749459D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.225592190D+05	-1.396782195D+03	1.403092409D+01	-4.098161770D-04	9.023845720D-08				
-1.032543966D-11	4.778671550D-16		-3.138889875D+04	-4.959121431D+01				

NaO Gurvich,1982 pt1 p318 pt2 p358.

2 tps82 NA	1.00O	1.00	0.00	0.00	0.00	0	38.9891700	106505.317
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.857748013D+04	-3.371497320D+02	5.644560020D+00	-3.136926368D-03	6.330775390D-06				
-5.429462470D-09	1.687183770D-12		1.320332678D+04	-4.996131150D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.569744011D+05	-2.269334161D+03	9.224397620D+00	-3.651269100D-03	1.446811119D-06				
-2.443068386D-10	1.428508328D-14		2.413239357D+04	-2.989159486D+01				

NaOH Gurvich,1996b.

2 g12/96 NA	1.00O	1.00H	1.00	0.00	0.00	0	39.9971100	-191000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.442036740D+04	-7.923218180D+02	8.997932300D+00	-4.079844520D-03	3.065783937D-06				
-5.119189340D-10	-1.541016409D-13		-2.086951091D+04	-2.510590090D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.753787760D+05	-2.342514649D+03	7.978469890D+00	1.016451512D-04	-6.268531950D-08				
1.022715136D-11	-5.713286410D-16		-9.509901710D+03	-2.202310401D+01				

NaOH+ Chase,1998 p1297 12/71. Jacox,1994.

3 g 2/01 NA	1.00O	1.00H	1.00E	-1.00	0.00	0	39.9965614	683862.371
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.278039363D+04	-6.672194220D+02	8.921593120D+00	-4.481263270D-03	3.951883920D-06				
-1.173341234D-09	2.041806631D-14		8.363382190D+04	-2.258912262D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.815413650D+05	-2.363159755D+03	8.053203930D+00	7.271279740D-05	-5.897417890D-08				
1.007487881D-11	-5.474406210D-16		9.584441650D+04	-2.079484012D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.839326542D+07	1.778338286D+04	2.821047612D+00	5.793749100D-04	-3.328793850D-08				
9.421248450D-13	-1.072317149D-17		-6.175194270D+04	2.465488033D+01				



## Appendix D (continued)

Na2 Gurvich,1982 pt1 p314 pt2 p357.  
 2 tpis82 NA 2.00 0.00 0.00 0.00 0.00 0 45.9795400 142339.125  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10403.125  
 6.848628680D+03-1.530836599D+02 5.325230390D+00-1.944906088D-03 2.657477888D-06  
 -9.096841120D-10-2.448756730D-13 1.649170574D+04-2.653564394D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10403.125  
 1.929940758D+07-6.269280120D+04 8.267682110D+01-4.565137810D-02 1.259515667D-05  
 -1.560445735D-09 7.024677170D-14 4.090820800D+05-5.509970890D+02

Na2Br2 Gurvich,1982 pt1 p342 pt2 p380.  
 2 tpis82 NA 2.00BR 2.00 0.00 0.00 0.00 0 205.7875400 -480848.453  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19591.547  
 -1.384946731D+04-1.573241177D+02 1.063192589D+01-1.383418339D-03 1.697156537D-06  
 -1.092992547D-09 2.870988020D-13 -6.010391820D+04-1.861473856D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19591.547  
 -3.021730975D+04-2.659232780D+00 1.000225819D+01-9.935490630D-07 2.358676253D-10  
 -2.857194816D-14 1.381909879D-18 -6.090039920D+04-1.494517863D+01

Na2CL2 Gurvich,1982 pt1 p338 pt2 p376.  
 2 tpis82 NA 2.00CL 2.00 0.00 0.00 0.00 0 116.8855400 -564401.783  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18699.327  
 -1.082955250D+04-3.139528641D+02 1.124411332D+01-2.697665795D-03 3.286359480D-06  
 -2.105377639D-09 5.508056610D-13 -6.938675430D+04-2.511011582D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18699.327  
 -4.412105230D+04-5.393491280D+00 1.000453407D+01-1.981155641D-06 4.680188200D-10  
 -5.648940680D-14 2.724721177D-18 -7.098063410D+04-1.787230397D+01

Na2F2 Gurvich,1982 pt1 p333 pt2 p372.  
 2 tpis82 NA 2.00F 2.00 0.00 0.00 0.00 0 83.9763464 -834062.776  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16682.330  
 2.351580802D+04-1.000737062D+03 1.375845076D+01-7.838346980D-03 9.276288700D-06  
 -5.813612970D-09 1.495354820D-12 -9.835831880D+04-4.381148090D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16682.330  
 -9.030750690D+04-1.893938035D+01 1.001535518D+01-6.539675450D-06 1.516333603D-09  
 -1.804877459D-13 8.613474920D-18 -1.034896664D+05-2.178860202D+01

Na2I2 Gurvich,1982 pt1 p346 pt2 p383.  
 2 tpis82 NA 2.00I 2.00 0.00 0.00 0.00 0 299.7884800 -356869.932  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20246.068  
 -1.305063983D+04-8.992506680D+01 1.036367976D+01-8.000070190D-04 9.848777980D-07  
 -6.359373120D-10 1.673774775D-13 -4.551465490D+04-1.487509548D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20246.068  
 -2.231236397D+04-1.515570558D+00 1.000129413D+01-5.715035380D-07 1.360287207D-10  
 -1.650916036D-14 7.996149680D-19 -4.596921750D+04-1.276523965D+01

Na2O Gurvich,1982 pt1 p321 pt2 p361.  
 2 tpis82 NA 2.00O 1.00 0.00 0.00 0.00 0 61.9789400 -16559.830  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14410.170  
 3.901149290D+04-7.266207890D+02 9.623710780D+00-3.556418640D-03 3.470704350D-06  
 -1.835177736D-09 4.062134710D-13 -4.593073250D+02-2.349565832D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14410.170  
 -6.600525160D+04-2.569021634D+01 7.519385420D+00-7.811635240D-06 1.735015890D-09  
 -1.996634558D-13 9.276433550D-18 -4.297339650D+03-1.063530214D+01

Na2O+ Gurvich,1982 pt1 p322 pt2 p362.  
 2 tpis82 NA 2.00O 1.00E -1.00 0.00 0.00 0 61.9783914 520833.968  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14606.568  
 2.647969755D+04-5.969062160D+02 9.294129530D+00-3.080702005D-03 3.080460653D-06  
 -1.669452593D-09 3.789784140D-13 6.347310250D+04-2.025274459D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14606.568  
 -5.740909330D+04-1.989178143D+01 7.515295260D+00-6.258333230D-06 1.407321045D-09  
 -1.635833952D-13 7.662445130D-18 6.032977470D+04-9.426526740D+00

Na2O2 Gurvich,1982 pt1 p324 pt2 p364.  
 2 tpis82 NA 2.00O 2.00 0.00 0.00 0.00 0 77.9783400 -123930.345  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15565.255  
 7.382458920D+04-1.355125340D+03 1.255579861D+01-2.112046045D-03 4.920353520D-08  
 1.003950603D-09-4.447732070D-13 -1.058858918D+04-4.021811780D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15565.255  
 -1.732295239D+05-1.137561118D+02 1.008529143D+01-3.422098940D-05 7.577721890D-09  
 -8.701256730D-13 4.036061390D-17 -1.780300574D+04-2.386789190D+01

## Appendix D (continued)

Na2O2H2 Gurvich, 1996b.

2 g 8/01 NA	2.000	2.00H	2.00	0.00	0.00	0.00	0	79.9942200	-624000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.089414289D+05	-2.634822704D+03	2.306608858D+01	-1.689310193D-02	1.673483190D-05					
-7.821166010D-09	1.475034470D-12		-6.593137330D+04	-9.802987580D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.675713839D+06	-4.704921170D+03	1.697343934D+01	1.961487616D-04	-1.236951748D-07					
2.025311778D-11	-1.132991623D-15		-4.856245570D+04	-6.813480980D+01					

Na2SO4 Gurvich, 1982 pt1 p349 pt2 p385.

2 tpi82 NA	2.00S	1.000	4.00	0.00	0.00	0	142.0421400	-1040132.302	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.344283210D+04	-1.210880769D+03	8.742353000D+00	3.600796630D-02	-5.117645960D-05					
3.481569040D-08	-9.321931220D-12		-1.217387045D+05	-2.061505785D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.754483110D+05	-9.817060340D+02	1.973310397D+01	-2.936395520D-04	6.498708170D-08					
-7.462479400D-12	3.462491660D-16		-1.270597762D+05	-7.667871596D+01					

Na3CL3 Gurvich, 1982 pt1 p339 pt2 p377.

2 tpi82 NA	3.00CL	3.00	0.00	0.00	0.00	0	175.3283100	-912674.509	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.254216670D+04	-5.502160460D+02	1.816110649D+01	-4.656515260D-03	5.646438220D-06					
-3.604760320D-09	9.405556240D-13		-1.119270172D+05	-5.290104960D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.160297970D+04	-9.573493810D+00	1.600799614D+01	-3.478356970D-06	8.190943690D-10					
-9.863210030D-14	4.749005350D-18		-1.147252948D+05	-4.031342160D+01					

Na3F3 Gurvich, 1982 pt1 p334 pt2 p373.

2 tpi82 NA	3.00F	3.00	0.00	0.00	0.00	0	125.9645196	-1348015.386	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.247030350D+04	-1.775597273D+03	2.250927609D+01	-1.333033615D-02	1.555790239D-05					
-9.646011460D-09	2.460254271D-12		-1.580736389D+05	-8.580122370D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.553995698D+05	-3.551970190D+01	1.602841159D+01	-1.198056094D-05	2.757248730D-09					
-3.263300970D-13	1.550483212D-17		-1.672141773D+05	-4.753780680D+01					

Nb Hf:Gurvich, 1982. Moore, 1971. Moore, 1970a. Gordon, 1999.

3 g 3/98 NB	1.00	0.00	0.00	0.00	0.00	0	92.9063800	723113.099	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.889660670D+04	-1.212813914D+03	1.034579819D+01	-1.676630056D-02	1.979119979D-05					
-1.218224409D-08	3.058098336D-12		9.165315140D+04	-3.594742850D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.096553196D+06	2.546650713D+03	2.236054882D+00	-1.280029198D-03	8.464237990D-07					
-1.486269508D-10	8.714309406D-15		6.879124550D+04	1.398169030D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.818626365D+09	-1.032414940D+06	2.308238005D+02	-2.445004311D-02	1.395626888D-06					
-4.087233010D-11	4.826490497D-16		8.359622560D+06	-1.997797290D+03					

Nb+ Moore, 1971. Moore, 1970a. Gordon, 1999.

3 g 7/97 NB	1.00E	-1.00	0.00	0.00	0.00	0	92.9058314	1393604.675	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.314447859D+05	-2.000135035D+03	1.505024212D+01	-2.996583942D-02	3.729868630D-05					
-2.269869569D-08	5.449089902D-12		1.760054029D+05	-6.224595520D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.077639646D+06	2.159046421D+03	2.310604767D+00	-5.363991760D-04	5.057915090D-07					
-1.032401533D-10	6.629241280D-15		1.517945546D+05	1.210678502D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.876113970D+07	-2.202847919D+04	1.427004521D+01	-2.295936786D-03	2.430819459D-07					
-1.116131589D-11	1.836221996D-16		3.245415600D+05	-8.494555710D+01					

Nb- Hotop, 1985. Gordon, 1999.

3 g 9/97 NB	1.00E	1.00	0.00	0.00	0.00	0	92.9069286	631054.008	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.220924850D+04	5.259501250D+02	3.470468390D+00	-4.950505530D-03	7.401859030D-06					
-5.016302070D-09	1.314100719D-12		7.178828870D+04	5.155510070D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.117458019D+05	1.340072834D+02	2.391474129D+00	4.524813430D-05	-1.025345000D-08					
1.195577988D-12	-5.606330450D-17		7.473996750D+04	9.675315610D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.279446680D+05	1.664265071D+02	2.463334336D+00	4.161717840D-06	-2.573750764D-10					
8.239892930D-15	-1.069096936D-19		7.430433860D+04	9.186188470D+00					

## Appendix D (continued)

NbCL5 Chase,1998 p918.

2 j12/74 NB	1.00CL	5.00	0.00	0.00	0.00	0.00	0.00	270.1713800	-703330.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.348277970D+04	-1.919172996D+03	2.290799567D+01	-1.404352774D-02	1.638106985D-05					
-1.018941843D-08	2.612266639D-12							-7.974118810D+04	-8.439637087D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.563816638D+05	-4.450521280D+01	1.603544630D+01	-1.489949737D-05	3.420777920D-09					
-4.041124420D-13	1.917266128D-17							-8.962815120D+04	-4.374582607D+01

NbO Gurvich,1982 pt1 p76 pt2 p78.

3 tpis82 NB	1.000	1.00	0.00	0.00	0.00	0.00	0	108.9057800	210988.706
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.797834360D+03	2.839767438D+02	5.645708400D-01	1.134928619D-02	-1.549821141D-05					
1.047624988D-08	-2.762937835D-12							2.317993893D+04	2.365708974D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.532258780D+05	-1.287669306D+03	4.980066040D+00	1.116014163D-04	4.031838680D-08					
1.048773710D-11	-1.893595022D-15							3.268457790D+04	-1.868958549D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.210846640D+07	-7.508889140D+04	3.023869608D+01	-2.881829240D-03	1.595446362D-07					
-4.532772640D-12	5.266479160D-17							5.788974420D+05	-2.169255418D+02

NbOCL3 Barin,1989. Wagman,1982.

2 bar 89 NB	1.000	1.00CL	3.00	0.00	0.00	0	215.2647800	-752300.000	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.108482359D+05	1.173066983D+02	1.165558433D+01	1.287422064D-03	-1.659778281D-06					
1.102107826D-09	-2.949903264D-13							-9.504023920D+04	-2.386450092D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.515551427D+05	5.305545230D+01	1.228915282D+01	-1.527366571D-04	6.778576440D-08					
-9.365170650D-12	4.670036930D-16							-9.490768120D+04	-2.745263834D+01

NbO2 Gurvich,1982 pt1 p80 pt2 p81.

2 tpis82 NB	1.000	2.00	0.00	0.00	0.00	0	124.9051800	-201266.752	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.739046582D+04	3.881029440D+01	9.024299120D-01	1.909523319D-02	-2.667013583D-05					
1.813901051D-08	-4.872365880D-12							-2.528518558D+04	2.289323379D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.851859900D+05	9.112249320D+02	6.339199840D+00	-8.230080300D-05	1.984439605D-07					
-3.261171490D-11	1.602430854D-15							-3.325027320D+04	3.559556550D+00

Ne Ref-Elm. Moore,1971. Moore,1970a. Gordon,1999.

3 g 5/97 NE	1.00	0.00	0.00	0.00	0.00	0	20.1797000	0.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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	3.355322720D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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	3.355322720D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.238252746D+07	6.958579580D+03	1.016709287D+00	1.424664555D-04	-4.803933930D-09					
-1.170213183D-13	8.415153652D-18							-5.663933630D+04	1.648438697D+01

Ne+ Moore,1971. Moore,1970a. Gordon,1999.

3 g 3/97 NE	1.00E	-1.00	0.00	0.00	0.00	0	20.1791514	2086965.946	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.281551480D+04	-8.695697990D+02	6.108646970D+00	-5.841356930D-03	5.041044170D-06					
-2.293759207D-09	4.339065680D-13							2.545996890D+05	-1.673449355D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.112742658D+05	4.765697970D+02	2.196650531D+00	1.102593151D-04	-2.287564425D-08					
2.510218183D-12	-1.126646096D-16							2.472536944D+05	7.466140540D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.615474110D+04	1.418980160D+02	2.475716842D+00	1.944430992D-06	-6.323099200D-11					
-1.313313446D-16	3.534699010D-20							2.494452217D+05	5.366882220D+00

Ni Hf:Hultgren,1973. Litzen,1993. Gordon,1999.

3 g 8/97 NI	1.00	0.00	0.00	0.00	0.00	0	58.6934000	430116.605	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.235810550D+04	6.015264620D+02	-1.079270657D+00	1.089505519D-02	-1.369578748D-05					
8.317725790D-09	-2.019206968D-12							4.813810810D+04	2.718829200D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.938262210D+05	1.092909991D+03	2.410485014D+00	-1.599071827D-05	-1.047414069D-08					
6.624795210D-12	-4.448865218D-17							4.336072170D+04	9.677195600D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.492669880D+08	-1.654227575D+05	3.349869360D+01	-3.527085900D-03	3.240060240D-07					
-1.604177606D-11	2.935430214D-16							1.409017848D+06	-2.672455567D+02

## Appendix D (continued)

Ni+ Sugar,1985. Gordon,1999.

3 g 8/97 NI	1.00E	-1.00	0.00	0.00	0.00	0	58.6928514	1172594.573
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6205.773
-8.969386030D+04	1.173601500D+03	-3.410620410D+00	1.390739137D-02	-1.501714923D-05				
7.896337900D-09	-1.648686761D-12		1.345589500D+05	4.031495160D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6205.773
-3.961999320D+06	1.017084853D+04	-6.029331290D+00	2.770858029D-03	-8.902077700D-08				
-5.541000580D-11	5.235342833D-15		7.340395120D+04	7.137503100D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6205.773
5.286662360D+07	-3.719827100D+04	1.470794435D+01	-1.489309517D-03	8.648712770D-08				
-1.705443550D-12	5.049635419D-18		4.253204090D+05	-9.590502160D+01				

Ni- Hotop,1985. Gordon,1999.

3 g 9/97 NI	1.00E	1.00	0.00	0.00	0.00	0	58.6939486	311764.357
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6207.157
-8.437624750D+04	1.135476552D+03	-3.380615830D+00	1.423003786D-02	-1.582586302D-05				
8.608840410D-09	-1.875316029D-12		3.124307590D+04	3.998061300D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6207.157
-5.433424800D+05	1.182645330D+03	2.126441240D+00	3.730455940D-05	6.953608430D-09				
-1.945719381D-12	1.271571579D-16		2.854759122D+04	1.043462235D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6207.157
2.235741343D+06	-7.539321100D+02	2.675777011D+00	-2.056834268D-05	1.297167360D-09				
-4.210909080D-14	5.520885950D-19		4.359114370D+04	5.724516640D+00				

NiCL Chase,1998 p794.

2 j 9/77 NI	1.00CL	1.00	0.00	0.00	0.00	0	94.1464000	182004.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9464.921
-2.357997085D+04	2.205491630D+02	2.714260287D+00	4.453598470D-03	-2.849162229D-06				
-1.691898007D-10	5.156699260D-13		1.957229490D+04	1.423643068D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9464.921
-3.905769190D+06	9.961533990D+03	-3.839432340D+00	2.767979391D-03	-7.005959380D-08				
-5.741403660D-11	5.307635800D-15		-4.505397050D+04	6.769402548D+01				

NiCL2 Chase,1998 p840.

2 j 9/77 NI	1.00CL	2.00	0.00	0.00	0.00	0	129.5994000	-73931.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								14206.546
7.109976530D+04	-1.218958288D+03	1.208750596D+01	-8.674403140D-03	1.043608104D-05				
-6.298493010D-09	1.485857653D-12		-5.006998710D+03	-3.499472036D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								14206.546
1.585889817D+05	-1.161488738D+03	9.608015380D+00	-9.461224510D-04	2.608172043D-07				
-3.264637250D-11	1.525950893D-15		-4.578985540D+03	-2.212397347D+01				

NiO Pedley,1983 p1012 p1019.

2 g12/00 NI	1.00O	1.00	0.00	0.00	0.00	0	74.6928000	297064.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8866.569
2.320630462D+04	-1.907136094D+02	3.190178620D+00	5.291383490D-03	-8.080210430D-06				
5.839812760D-09	-1.639499596D-12		3.576711120D+04	7.841265670D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								8866.569
-7.234091940D+04	-8.035554270D+01	4.559221020D+00	2.305154510D-05	5.139832820D-09				
-5.853474910D-13	2.697077329D-17		3.461143850D+04	1.209414814D+00				

NiS Chase,1998 p1707.

2 j12/76 NI	1.00S	1.00	0.00	0.00	0.00	0	90.7584000	357419.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9218.527
-1.272488974D+04	1.432801381D+02	2.471951556D+00	5.505271120D-03	-3.418355280D-06				
-3.099052241D-10	6.268154670D-13		4.117716080D+04	1.517981835D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								9218.527
-7.358128980D+05	1.178231095D+03	4.837865580D+00	-3.931201390D-04	1.341974852D-07				
-1.569591708D-11	6.677045060D-16		3.275565940D+04	3.690652283D+00				

O D0(O2):Brix,1954. Moore,1976. Gordon,1999.

3 g 5/97 O	1.00	0.00	0.00	0.00	0.00	0	15.9994000	249175.003
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6725.403
-7.953611300D+03	1.607177787D+02	1.966226438D+00	1.013670310D-03	-1.110415423D-06				
6.517507500D-10	-1.584779251D-13		2.840362437D+04	8.404241820D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6725.403
2.619020262D+05	-7.298722030D+02	3.317177270D+00	-4.281334360D-04	1.036104594D-07				
-9.438304330D-12	2.725038297D-16		3.392428060D+04	-6.679585350D-01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								6725.403
1.779004264D+08	-1.082328257D+05	2.810778365D+01	-2.975232262D-03	1.854997534D-07				
-5.796231540D-12	7.191720164D-17		8.890942630D+05	-2.181728151D+02				

## Appendix D (continued)

O+                    Martin,1993. Gordon,1999.

3 g 8/97 O	1.00E -1.00	0.00	0.00	0.00	0.00	0.00	15.9988514	1568787.228
298.150	1000.0007 -2.0 -1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						1.879352842D+05	4.393376760D+00
1000.000	6000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	6197.428
-2.166513208D+05	6.665456150D+02	1.702064364D+00	4.714992810D-04	-1.427131823D-07				
2.016595903D-11	-9.107157762D-16		1.837191966D+05	1.005690382D+01				
6000.000	20000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	6197.428
-2.143835383D+08	1.469518523D+05	-3.680864540D+01	5.036164540D-03	-3.087873854D-07				
9.186834870D-12	-1.074163268D-16		-9.614208960D+05	3.426193080D+02				

O-                    Gurvich,1989 pt1 p93. Hotop,1985. Gordon,1999.

3 g 1/97 O	1.00E 1.00	0.00	0.00	0.00	0.00	0.00	15.9999486	101846.192
298.150	1000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	6570.792
-5.695857110D+03	1.099287334D+02	2.184719661D+00	5.326359800D-04	-5.298878440D-07				
2.870216236D-10	-6.524692740D-14		1.093287498D+04	6.729863860D+00				
1000.000	6000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	6570.792
9.769363180D+03	7.159604780D+00	2.494961726D+00	1.968240938D-06	-4.304174850D-10				
4.912083080D-14	-2.271600083D-18		1.149554438D+04	4.837036440D+00				
6000.000	20000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	6570.792
5.662391000D+02	7.572340320D+00	2.498352500D+00	1.862632395D-07	-1.151227211D-11				
3.688814210D-16	-4.793297600D-21		1.148426000D+04	4.813406590D+00				

OD                    D0(OH)with ZPEadj. Gurvich,1989 pt1 p135 pt2 p47.

2 g 4/02 O	1.00D 1.00	0.00	0.00	0.00	0.00	0.00	18.0135020	35172.008
200.000	1000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8999.108
2.118691536D+04	-2.785982360D+02	5.456210120D+00	-6.148119830D-03	9.117670560D-06				
-5.527812710D-09	1.239794711D-12		4.464878250D+03	-7.616618910D+00				
1000.000	6000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8999.108
7.832473160D+05	-2.532992554D+03	5.952124650D+00	-3.743595280D-04	4.959527620D-08				
3.454454730D-12	-7.380626800D-16		1.930492973D+04	-1.568898441D+01				

OD-                    Gurvich,1989 pt1 p137 pt2 p48.

2 g 4/02 O	1.00D 1.00E 1.00	0.00	0.00	0.00	0.00	0.00	18.0140506	-147557.896
298.150	1000.000 7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8642.104
5.606128320D+04	-7.514156150D+02	7.544188470D+00	-1.092083064D-02	1.503688938D-05				
-9.351665840D-09	2.246466046D-12	0.000000000D+00	-1.515707370D+04	-2.106498377D+01				
1000.000	6000.000 7 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8642.104
3.029467029D+05	-1.079684654D+03	4.211417380D+00	6.260830070D-04	-2.411665054D-07				
4.248425540D-11	-2.387099102D-15	0.000000000D+00	-1.188935343D+04	-4.724898790D+00				

OH                    D0(H-OH): Ruscic,2002. Gurvich,1978 pt1 p110 pt2 p37.

3 g 4/02 O	1.00H 1.00	0.00	0.00	0.00	0.00	0.00	17.0073400	37278.206
200.000	1000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8813.106
-1.998858990D+03	9.300136160D+01	3.050854229D+00	1.529529288D-03	-3.157890998D-06				
3.315446180D-09	-1.138762683D-12		2.991214235D+03	4.674110790D+00				
1000.000	6000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8813.106
1.017393379D+06	-2.509957276D+03	5.116547860D+00	1.305299930D-04	-8.284322260D-08				
2.006475941D-11	-1.556993656D-15		2.019640206D+04	-1.101282337D+01				
6000.000	20000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8813.106
2.847234193D+08	-1.859532612D+05	5.008240900D+01	-5.142374980D-03	2.875536589D-07				
-8.228817960D-12	9.567229020D-17		1.468393908D+06	-4.023555580D+02				

OH+                    IP: Wiedmann,1992. Gurvich,1978 v1 pt2 p39.

3 g 4/02 O	1.00H 1.00E -1.00	0.00	0.00	0.00	0.00	0.00	17.0067914	1299213.203
298.150	1000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8603.103
6.031630860D+04	-7.573520300D+02	7.307752930D+00	-9.506881670D-03	1.202555795D-05				
-6.829026100D-09	1.501588659D-12		1.589262158D+05	-1.950106996D+01				
1000.000	6000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8603.103
5.040729100D+05	-1.380052958D+03	4.125462200D+00	8.331948840D-04	-3.442856290D-07				
6.792853950D-11	-4.363872130D-15		1.643839235D+05	-3.997058490D+00				
6000.000	20000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8603.103
1.158286700D+09	-6.841280390D+05	1.576194558D+02	-1.618421339D-02	8.846128780D-07				
-2.475038507D-11	2.807730875D-16		5.616597180D+06	-1.351879042D+03				

OH-                    Gurvich,1989 pt1 p118 pt2 p32.

2 g 4/02 O	1.00H 1.00E 1.00	0.00	0.00	0.00	0.00	0.00	17.0078886	-145256.196
298.150	1000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8606.104
2.910880827D+04	-3.216904940D+02	4.851029050D+00	-2.579035357D-03	2.004980024D-06				
-7.956852960D-11	-2.320495634D-13		-1.688886234D+04	-7.121591300D+00				
1000.000	6000.0007 -2.0 -1.0	0.0	1.0	2.0	3.0	4.0	0.0	8606.104
4.711331170D+05	-8.572336690D+02	3.166181210D+00	1.233581296D-03	-3.999244580D-07				
6.239081670D-11	-3.354343220D-15		-1.224849139D+04	1.487736260D+00				

## Appendix D (continued)

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		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-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	8.193346705D-16		-1.689010929D+04	1.738716506D+01							
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		8680.104
4.975294300D+08	-2.866106874D+05	6.690352250D+01	-6.169959020D-03	3.016396027D-07							
-7.421416600D-12	7.278175770D-17		2.293554027D+06	-5.530621610D+02							

O2+                      Gurvich,1989 pt1 p98 pt2 p11.

3	tpis89	O	2.00E	-1.00	0.00	0.00	0.00	0	31.9982514	1171828.436	
	298.150		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.607205450D+04	1.051875934D+03	-5.432380470D-01	6.571166540D-03	-3.274263750D-06							
5.940645340D-11	3.238784790D-13		1.345544668D+05	2.902709750D+01							
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		9311.112
7.384654880D+04	-8.459559540D+02	4.985164160D+00	-1.611010890D-04	6.427083990D-08							
-1.504939874D-11	1.578465409D-15		1.446321044D+05	-5.811230650D+00							
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		9311.112
-1.562125524D+09	1.161406778D+06	-3.302504720D+02	4.710937520D-02	-3.354461380D-06							
1.167968599D-10	-1.589754791D-15		-8.857866270D+06	2.852035602D+03							

O2-                      Gurvich,1989 pt1 p100 pt2 p13.

2	g11/99	O	2.00E	1.00	0.00	0.00	0.00	0	31.9993486	-48027.921	
	298.150		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.883874344D+04	1.149551768D+02	1.518876821D+00	8.016111380D-03	-9.850571030D-06							
6.044196210D-09	-1.486439845D-12		-7.101538760D+03	1.501210380D+01							
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		9349.611
-5.655208050D+04	-2.367815862D+02	4.675833670D+00	-2.197245300D-05	1.711509280D-08							
-1.757645062D-12	8.248172790D-17		-5.960177750D+03	-2.436885556D+00							

O3                      Gurvich,1989 pt1 p101 pt2 p15.

2	g	8/01	O	3.00	0.00	0.00	0.00	0	47.9982000	141800.000	
	200.000		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.282314507D+04	5.898216640D+02	-2.547496763D+00	2.690121526D-02	-3.528258340D-05							
2.312290922D-08	-6.044893270D-12		1.348368701D+04	3.852218580D+01							
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		10366.305
-3.869662480D+07	1.023344994D+05	-8.961551600D+01	3.706144970D-02	-4.137638740D-06							
-2.725018591D-10	5.248188110D-14		-6.517918180D+05	7.029109520D+02							

P                      Hf:Cox,1989. Martin,1985. Gordon,1999.

3	g	5/97	P	1.00	0.00	0.00	0.00	0	30.9737610	316500.000	
	200.000		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.040866570D+01	-7.639418650D-01	2.504563992D+00	-1.381689958D-05	2.245585515D-08							
-1.866399889D-11	6.227063395D-15		3.732421910D+04	5.359303481D+00							
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		6197.428
1.261794642D+06	-4.559838190D+03	8.918079310D+00	-4.381401460D-03	1.454286224D-06							
-2.030782763D-10	1.021022887D-14		6.541723960D+04	-3.915974795D+01							
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		6197.428
-2.215392545D+07	-4.566911180D+04	2.837245428D+01	-4.483244040D-03	3.579413080D-07							
-1.255311557D-11	1.590290483D-16		3.370905760D+05	-2.056960928D+02							

P+                      Martin,1985. Gordon,1999.

3	g	4/97	P	1.00E	-1.00	0.00	0.00	0	30.9732124	1336453.460	
	298.150		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.316908110D+04	9.627979140D+02	-3.693938050D-01	4.766778340D-03	-4.574768580D-06							
2.371262331D-09	-5.131314900D-13		1.549406849D+05	2.376640762D+01							
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		8141.860
-5.594249360D+05	1.722576545D+03	8.430381090D-01	6.287368940D-04	-6.317195460D-08							
-1.810842484D-12	4.318112570D-16		1.490493431D+05	1.845275207D+01							
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		8141.860
1.362531054D+07	-8.717502380D+03	4.747426280D+00	-1.620871933D-04	-3.935548100D-10							
4.845613020D-13	-7.448402970D-18		2.284649718D+05	-1.346454894D+01							

P-                      Hotop,1985. Gordon,1999.

3	g	4/97	P	1.00E	1.00	0.00	0.00	0	30.9743096	238826.765	
	298.150		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.008949093D+04	1.826468403D+02	1.962456304D+00	9.197377540D-04	-9.214998630D-07							
5.012872360D-10	-1.142677121D-13		2.703082432D+04	9.478137822D+00							
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		6747.865
1.543488016D+04	9.495009340D+00	2.493170861D+00	2.700167711D-06	-5.949210390D-10							
6.823766290D-14	-3.166959910D-18		2.797572693D+04	6.246793872D+00							
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0		6747.865
1.724147889D+03	1.074832503D+01	2.497654940D+00	2.655333078D-07	-1.642839012D-11							
5.268015350D-16	-6.849362660D-21		2.795482976D+04	6.215849262D+00							

## Appendix D (continued)

PCL Gurvich,1989 pt1 p431 pt2 p282.

2 tps89 P	1.00CL	1.00	0.00	0.00	0.00	0	66.4267610	134615.112
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.488861700D+04	-5.603119340D+02	6.264568480D+00	-3.183364370D-03	3.495326840D-06				
-2.091034291D-09	5.418758600D-13			1.774653764D+04	-8.074572148D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.471681510D+05	9.935557930D+02	3.399430270D+00	4.019711700D-04	8.295588390D-08				
-3.090212484D-11	2.106384858D-15			8.433591150D+03	1.064902238D+01			

PCL2 Gurvich,1989 pt1 p432 pt2 p283.

2 tps89 P	1.00CL	2.00	0.00	0.00	0.00	0	101.8797610	-54292.353
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.190084500D+04	-1.060904200D+03	1.058549940D+01	-6.879917530D-03	7.620773180D-06				
-4.530115470D-09	1.116671660D-12			-3.220331180D+03	-2.753518359D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.349833970D+04	-2.625249470D+01	7.020361810D+00	-8.388768680D-06	1.896784740D-09				
-2.214879920D-13	1.041653550D-17			-8.742993680D+03	-6.234023190D+00			

PCL2- Gurvich,1989 pt1 p433 pt2 p284.

2 tps89 P	1.00CL	2.00E	1.00	0.00	0.00	0	101.8803096	-356285.253
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.934832770D+04	-9.601590540D+02	9.884769700D+00	-4.950202950D-03	4.946217870D-06				
-2.678675201D-09	6.076723610D-13			-3.998072400D+04	-2.413131695D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.564986760D+04	-3.185555940D+01	7.024494960D+00	-1.002251172D-05	2.253747944D-09				
-2.619657192D-13	1.227059658D-17			-4.503811430D+04	-6.721522361D+00			

PCL3 Gurvich,1989 pt1 p433 pt2 p285.

2 tps89 P	1.00CL	3.00	0.00	0.00	0.00	0	137.3327610	-289500.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.717745470D+04	-1.617650860D+03	1.536080470D+01	-1.011077050D-02	1.103408340D-05				
-6.476121020D-09	1.579151140D-12			-2.955893640D+04	-5.244338688D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.333076930D+05	-4.145883210D+01	1.003186060D+01	-1.301946160D-05	2.922916890D-09				
-3.391869240D-13	1.586425530D-17			-3.800336680D+04	-2.050737678D+01			

PCL5 Gurvich,1989 pt1 p435 pt2 p286.

2 tps89 P	1.00CL	5.00	0.00	0.00	0.00	0	208.2387610	-376000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.029070200D+05	-2.515707460D+03	2.430114970D+01	-1.564610690D-02	1.709873030D-05				
-1.006011430D-08	2.460158790D-12			-3.722582370D+04	-9.816335170D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.255906890D+05	-6.938542820D+01	1.605359630D+01	-2.202156960D-05	4.971392290D-09				
-5.799860050D-13	2.725970770D-17			-5.034234220D+04	-4.872454870D+01			

PF Gurvich,1989 pt1 p425 pt2 p276.

2 tps89 P	1.00F	1.00	0.00	0.00	0.00	0	49.9721642	-47944.793
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.227866728D+04	-1.727508706D+02	3.085366934D+00	5.489718230D-03	-8.247972540D-06				
5.868882910D-09	-1.617252113D-12			-5.809279650D+03	7.709718850D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.132572282D+06	3.200038550D+03	7.780502370D-01	1.969518902D-03	-4.365818970D-07				
5.243648570D-11	2.618755712D-15			-2.766773009D+04	2.759312302D+01			

PF+ Chase,1998 p1086.

3 j 6/77 P	1.00F	1.00E	-1.00	0.00	0.00	0	49.9716156	901518.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.779138157D+04	3.909991270D+02	1.257434156D+00	7.861363750D-03	-9.342312680D-06				
5.630915650D-09	-1.370669924D-12			1.054873882D+05	1.901676576D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.011525180D+04	-1.597504413D+02	4.621397480D+00	-2.378072183D-05	1.431831329D-08				
-2.300109157D-12	1.694069882D-16			1.078633756D+05	-4.072343950D-02			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.628686921D+07	1.300876535D+04	2.564713658D+00	3.269650350D-05	1.867188317D-08				
-9.293307220D-13	1.456723674D-17			-2.640503508D+02	1.921588661D+01			

PF- Chase,1998 p1087.

3 j 6/77 P	1.00F	1.00E	1.00	0.00	0.00	0	49.9727128	-164046.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.705210950D+03	-1.152432706D+02	4.254952310D+00	1.163521526D-03	-1.627947259D-06				
1.084382815D-09	-2.809490132D-13			-2.035558966D+04	2.217923793D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.303793388D+05	2.715526386D+02	4.137619810D+00	2.728610614D-04	-7.644416250D-08				
1.182073001D-11	-6.083906640D-16			-2.290799827D+04	3.748526100D+00			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.589702487D+07	2.274827883D+04	-2.913204829D+00	1.134351740D-03	-7.184766090D-08				
2.254067861D-12	-2.781608692D-17			-1.940751937D+05	6.372454240D+01			

## Appendix D (continued)

PFCL Gurvich,1989 pt1 p437 pt2 p288.

2 tpi89 P	1.00F	1.00CL	1.00	0.00	0.00	0	85.4251642	-283184.119
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.490188530D+04	-8.658679480D+02	7.944467650D+00	9.503779100D-04	-3.339090210D-06				
3.023977817D-09	-9.450377540D-13		-3.132843217D+04	-1.440426886D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.282143211D+05	-9.739043550D+01	7.072661660D+00	-2.903614134D-05	6.408504490D-09				
-7.338993770D-13	3.396723170D-17		-3.600649260D+04	-7.626493035D+00				

PFCL- Gurvich,1989 pt1 p438 pt2 p289.

2 tpi89 P	1.00F	1.00CL	1.00E	1.00	0.00	0	85.4257128	-529269.107
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.934336850D+04	-1.266972513D+03	9.912194530D+00	-3.877928300D-03	3.036692411D-06				
-1.296559380D-09	2.324226580D-13		-5.894505710D+04	-2.617050460D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.231565150D+05	-9.765861110D+01	7.074029570D+00	-2.997070692D-05	6.685280620D-09				
-7.722262200D-13	3.599382300D-17		-6.558817220D+04	-8.208878059D+00				

PFCL2 Gurvich,1989 pt1 p440 pt2 p292.

2 tpi89 P	1.00F	1.00CL	2.00	0.00	0.00	0	120.8781642	-511925.340
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.266560560D+04	-1.512138928D+03	1.303404207D+01	-2.903247162D-03	7.836652970D-07				
6.458340660D-10	-3.737641820D-13		-5.644237870D+04	-4.100905668D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.864589813D+05	-1.148004379D+02	1.008599754D+01	-3.447456520D-05	7.627972010D-09				
-8.753097430D-13	4.057788350D-17		-6.450472190D+04	-2.174054563D+01				

PFCL4 Gurvich,1989 pt1 p442 pt2 p295.

2 tpi89 P	1.00F	1.00CL	4.00	0.00	0.00	0	191.7841642	-635016.440
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.412071573D+05	-2.882471080D+03	2.387345233D+01	-1.239510207D-02	1.141290085D-05				
-5.705483820D-09	1.195229703D-12		-6.613478650D+04	-9.859693550D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.954375880D+05	-1.325154294D+02	1.610005380D+01	-4.035359170D-05	8.971130740D-09				
-1.033288810D-12	4.804468350D-17		-8.135719400D+04	-5.062403920D+01				

PF2 Gurvich,1989 pt1 p426 pt2 p277.

2 tpi89 P	1.00F	2.00	0.00	0.00	0.00	0	68.9705674	-513103.659
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.524765720D+04	-6.280517800D+02	5.137437920D+00	9.120673350D-03	-1.468773760D-05				
1.081268450D-08	-3.064944490D-12		-5.977541470D+04	-1.689589472D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.708467120D+05	-1.692051540D+02	7.125491600D+00	-4.990852850D-05	1.097335230D-08				
-1.252870260D-12	5.784791140D-17		-6.338295840D+04	-1.041715673D+01				

PF2- Gurvich,1989 pt1 p426 pt2 p278.

2 tpi89 P	1.00F	2.00E	1.00	0.00	0.00	0	68.9711160	-709337.947
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.404793057D+05	-1.699945753D+03	1.036823971D+01	-3.599587690D-03	1.961925800D-06				
-3.829329870D-10	-3.375549520D-14		-7.810434510D+04	-3.217375182D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.653976056D+05	-1.640604822D+02	7.124091520D+00	-5.015431400D-05	1.117302152D-08				
-1.289308601D-12	6.004706670D-17		-8.700223320D+04	-1.109074866D+01				

PF2CL Gurvich,1989 pt1 p439 pt2 p290.

2 tpi89 P	1.00F	2.00CL	1.00	0.00	0.00	0	104.4235674	-735076.682
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.397590160D+04	-1.318075883D+03	1.017203515D+01	5.571231220D-03	-1.100920478D-05				
8.726383180D-09	-2.567714099D-12		-8.381656170D+04	-2.766012951D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.409281185D+05	-2.033484670D+02	1.015150769D+01	-6.048367310D-05	1.333942001D-08				
-1.526772528D-12	7.063339180D-17		-9.101110590D+04	-2.417825549D+01				

PF2CL3 Gurvich,1989 pt1 p442 pt2 p294.

2 tpi89 P	1.00F	2.00CL	3.00	0.00	0.00	0	175.3295674	-878744.962
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.842099543D+05	-3.334402390D+03	2.388510873D+01	-1.030943175D-02	7.356504220D-06				
-2.498621785D-09	2.513997646D-13		-9.279549890D+04	-1.027991502D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.655272540D+05	-2.029694160D+02	1.615238015D+01	-6.118796570D-05	1.355610375D-08				
-1.557129640D-12	7.224359970D-17		-1.104941533D+05	-5.387308191D+01				



## Appendix D (continued)

PF3 Gurvich,1989 pt1 p427 pt2 p279.

2 tpris89 P	1.00F	3.00	0.00	0.00	0.00	0.00	0	87.9689706	-957400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.480984480D+04	-1.102340691D+03	7.160715110D+00	1.438278338D-02	-2.318137222D-05					
1.702244315D-08	-4.810991950D-12		-1.111837495D+05	-1.457652362D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.957040675D+05	-2.997689931D+02	1.022297023D+01	-8.890263450D-05	1.958901359D-08					
-2.240491075D-12	1.035952523D-16		-1.173743464D+05	-2.777419177D+01					

PF3CL2 Gurvich,1989 pt1 p441 pt2 p293.

2 tpris89 P	1.00F	3.00CL	2.00	0.00	0.00	0	158.8749706	-1122022.916
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.822497206D+05	-3.089610245D+03	2.067710388D+01	-1.168732391D-03	-5.020540740D-06				
5.804573350D-09	-1.965367906D-12		-1.228120667D+05	-8.627977355D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.223838050D+05	-3.207965220D+02	1.624013000D+01	-9.623655310D-05	2.129279712D-08				
-2.443515401D-12	1.132904350D-16		-1.392642151D+05	-5.531285745D+01				

PF4CL Gurvich,1989 pt1 p439 pt2 p291.

2 tpris89 P	1.00F	4.00CL	1.00	0.00	0.00	0	142.4203738	-1364909.395
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.804240323D+05	-2.741096618D+03	1.680192838D+01	9.919315250D-03	-2.025636171D-05				
1.617979147D-08	-4.772611520D-12		-1.532382587D+05	-6.679119965D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.781140040D+05	-4.264812830D+02	1.631812121D+01	-1.271374903D-04	2.806715254D-08				
-3.215166300D-12	1.488512118D-16		-1.680488362D+05	-5.735844805D+01				

PF5 Gurvich,1989 pt1 p429 pt2 p280.

2 tpris89 P	1.00F	5.00	0.00	0.00	0.00	0	125.9657770	-1593300.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.855778473D+05	-2.436979828D+03	1.201012406D+01	2.339343049D-02	-3.813944410D-05				
2.796136412D-08	-7.870704880D-12		-1.814566568D+05	-4.486488740D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.668727840D+05	-6.677917910D+02	1.649789569D+01	-1.990099440D-04	4.395007100D-08				
-5.036849540D-12	2.332945909D-16		-1.944321623D+05	-6.261721040D+01				

PH Gurvich,1989 pt1 p420 pt2 p272.

2 tpris89 P	1.00H	1.00	0.00	0.00	0.00	0	31.9817010	230752.104
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.273633198D+05	-3.972674060D+02	6.233697660D+00	-9.181784600D-03	1.523328123D-05				
-1.085888585D-08	2.929760547D-12		2.852768404D+04	-1.095191197D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.814730650D+05	-3.038451204D+03	7.467481020D+00	-1.837522255D-03	7.165947700D-07				
-1.142128853D-10	6.175410560D-15		4.536260180D+04	-2.467298140D+01				

PH2 Gurvich,1989 pt1 p422 pt2 p273.

2 tpris89 P	1.00H	2.00	0.00	0.00	0.00	0	32.9896410	119553.470
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.555268372D+04	-1.841602025D+02	4.895896040D+00	-3.495436600D-03	1.053418945D-05				
-8.377562920D-09	2.270766150D-12		1.409839468D+04	-2.210564792D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.127884913D+06	-4.715238250D+03	1.021498300D+01	-1.167573820D-03	2.150542671D-07				
-1.624213739D-11	3.766225240D-16		4.183074630D+04	-4.231623250D+01				

PH2- Gurvich,1989 pt1 p423 pt2 p274.

2 tpris89 P	1.00H	2.00E	1.00	0.00	0.00	0	32.9901896	-9265.418
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.950684490D+04	-7.719162910D+02	7.383537620D+00	-8.522947210D-03	1.474476507D-05				
-9.847160810D-09	2.413107871D-12		1.582295850D+03	-1.761306419D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.382525815D+06	-5.213400670D+03	1.021694832D+01	-1.116316349D-03	2.215004171D-07				
-2.338005187D-11	1.015580932D-15		2.990683733D+04	-4.378711585D+01				

PH3 Chase,1998 p1348.

2 j 6/62 P	1.00H	3.00	0.00	0.00	0.00	0	33.9975810	5439.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.384325340D+03	4.057567410D+02	-1.565680086D-01	1.338380613D-02	-8.275391430D-06				
3.024360831D-09	-6.421764630D-13		-2.159842124D+03	2.385561888D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.334801106D+06	-6.725463520D+03	1.445857073D+01	-1.639736883D-03	3.409218570D-07				
-3.736272080D-11	1.672947506D-15		3.910325710D+04	-7.198781190D+01				

## Appendix D (continued)

PN Gurvich,1989 pt1 p446 pt2 p299.

2 tps89 P	1.00N	1.00	0.00	0.00	0.00	0.00	0	44.9804610	171487.305
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.103203840D+04	8.202926680D+02	-1.392772765D+00	1.287989789D-02	-1.401425371D-05					
7.775633460D-09	-1.751539330D-12		1.573226520D+04	3.251070633D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.495625593D+05	1.760438830D+02	4.144121960D+00	2.478018097D-04	-5.674896300D-08					
4.263645120D-12	3.063920924D-16		1.770317267D+04	1.325517397D+00					

PO Gurvich,1989 pt1 p404 pt2 p258.

2 tps89 P	1.000	1.00	0.00	0.00	0.00	0	46.9731610	-27857.687	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.845754060D+04	1.141295708D+03	-2.779556060D+00	1.678458047D-02	-1.974879516D-05					
1.192602320D-08	-2.927460912D-12		-9.847745040D+03	4.184328297D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.36667440D+05	6.229355840D+02	3.565605460D+00	6.516620720D-04	-2.061770841D-07					
3.184413230D-11	-1.573691908D-15		-8.939790390D+03	6.954859188D+00					

PO- Gurvich,1989 pt1 p407 pt2 p259.

2 tps89 P	1.000	1.00E	1.00	0.00	0.00	0	46.9737096	-140067.094	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.434346320D+04	-4.123623550D+02	3.746483880D+00	3.858636470D-03	-5.963343040D-06					
4.278286360D-09	-1.139722989D-12		-1.555810937D+04	3.404436468D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.480294780D+02	3.470544870D+02	2.877890167D+00	1.622182445D-03	-4.870190990D-07					
6.645752270D-11	-3.395703760D-15		-1.987209540D+04	1.075444355D+01					

POCL3 Gurvich,1989 pt1 p436 pt2 p287.

2 tps89 P	1.000	1.00CL	3.00	0.00	0.00	0	153.3321610	-568400.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.793788160D+04	-1.270388280D+03	1.367716460D+01	1.082672100D-03	-1.736104060D-06					
8.460890640D-10	-1.174661330D-13		-6.507571880D+04	-4.314705941D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.185937970D+05	-5.080269680D+02	1.337784650D+01	-1.510731050D-04	3.340986780D-08					
-3.835329760D-12	1.779329880D-16		-7.009315090D+04	-3.984746301D+01					

POFCL2 Gurvich,1989 pt1 p444 pt2 p297.

2 tps89 P	1.000	1.00F	1.00CL	2.00	0.00	0	136.8775642	-793889.312	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.694061560D+04	-1.069242600D+03	1.071284279D+01	9.491183300D-03	-1.306412424D-05					
8.426906020D-09	-2.140294969D-12		-9.274894990D+04	-2.815077719D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.707647503D+05	-6.556502270D+02	1.348668421D+01	-1.942765035D-04	4.291184490D-08					
-4.921844800D-12	2.282079808D-16		-9.654392140D+04	-4.164963494D+01					

POF2CL Gurvich,1989 pt1 p443 pt2 p296.

2 tps89 P	1.000	1.00F	2.00CL	1.00	0.00	0	120.4229674	-1022607.040	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.226438160D+04	-9.691037700D+02	7.963635980D+00	1.755599796D-02	-2.398693997D-05					
1.572376747D-08	-4.079746000D-12		-1.202656893D+05	-1.593967075D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.347086590D+05	-8.176104810D+02	1.360664320D+01	-2.420426112D-04	5.343712720D-08					
-6.126461350D-12	2.839570116D-16		-1.233401194D+05	-4.496103437D+01					

POF3 Gurvich,1989 pt1 p430 pt2 p281.

2 tps89 P	1.000	1.00F	3.00	0.00	0.00	0	103.9683706	-1252000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.966030710D+04	-4.276705750D+02	3.669146100D+00	2.839493780D-02	-3.768318000D-05					
2.449104540D-08	-6.341972870D-12		-1.501124530D+05	5.160417996D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.690602420D+05	-1.005552540D+03	1.374529940D+01	-2.971037110D-04	6.554526640D-08					
-7.509987330D-12	3.478969910D-16		-1.499761730D+05	-4.882214181D+01					

PO2 Gurvich,1989 pt1 p408 pt2 p260.

2 tps89 P	1.000	2.00	0.00	0.00	0.00	0	62.9725610	-281527.237	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.372698220D+04	1.036741044D+03	-2.877797967D+00	2.278134083D-02	-2.567920328D-05					
1.465060412D-08	-3.387996700D-12		-3.993544720D+04	4.425309380D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.926210990D+05	-2.605465745D+03	9.517605610D+00	-1.180371565D-03	2.532912819D-07					
-1.789964539D-11	1.800381054D-16		-2.028884763D+04	-2.969743125D+01					

## Appendix D (continued)

PO2- Gurvich,1989 pt1 p409 pt2 p261.

2 tpris89 P	1.000	2.00E	1.00	0.00	0.00	0	62.9731096	-597623.751
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
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
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				

PS Gurvich,1989 pt1 p444 pt2 p298.

2 tpris89 P	1.00S	1.00	0.00	0.00	0.00	0	63.0387610	150431.316
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.689786800D+02	-4.637824070D+01	4.104649170D+00	1.555262273D-03	-2.315757288D-06				
1.661425178D-09	-4.631238400D-13		1.707875808D+04	4.230652171D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.702729081D+05	8.883548220D+02	3.169190120D+00	1.022480817D-03	-3.803740480D-07				
7.019861880D-11	-4.269122310D-15		1.121510462D+04	1.147334049D+01				

P2 Gurvich,1989 pt1 p398 pt2 p255.

2 tpris89 P	2.00	0.00	0.00	0.00	0.00	0	61.9475220	144000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.053922510D+04	-3.246177590D+02	4.022463810D+00	3.232094790D-03	-5.511052450D-06				
4.195572930D-09	-1.215032180D-12		1.796910870D+04	1.645350331D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.806936490D+05	2.307910870D+03	1.411743130D+00	2.108237420D-03	-7.360856620D-07				
-1.259360120D-10	-7.079752490D-15		1.329824740D+03	2.169741365D+01				

P2O3 Gurvich,1989 pt1 p410 pt2 p262.

2 tpris89 P	2.000	3.00	0.00	0.00	0.00	0	109.9457220	-684645.274
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.645753890D+04	7.580900550D+02	9.888436770D-01	2.859878730D-02	-3.231142110D-05				
1.834525170D-08	-4.212489300D-12		-8.820036740D+04	2.689914458D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.175344110D+05	-1.369902000D+03	1.401142960D+01	-4.023856960D-04	8.868345780D-08				
-1.015657280D-11	4.704356060D-16		-7.922757000D+04	-4.739487232D+01				

P2O4 Gurvich,1989 pt1 p411 pt2 p263.

2 tpris89 P	2.000	4.00	0.00	0.00	0.00	0	125.9451220	-933754.627
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.376091260D+04	4.905102830D+02	9.643649370D-01	3.886073580D-02	-4.675509220D-05				
2.812625630D-08	-6.824406100D-12		-1.168997790D+05	2.379582767D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.670114860D+05	-1.638423730D+03	1.721188610D+01	-4.826580150D-04	1.064461900D-07				
-1.219610070D-11	5.650654580D-16		-1.090435930D+05	-6.714276593D+01				

P2O5 Gurvich,1989 pt1 p411 pt2 p264.

2 tpris89 P	2.000	5.00	0.00	0.00	0.00	0	141.9445220	-1124370.354
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.999159220D+04	-4.594506590D+01	6.987486830D+00	2.883302970D-02	-3.104509530D-05				
1.643868680D-08	-3.467942300D-12		-1.381901400D+05	-3.400572711D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.247080160D+05	-2.016975080D+03	2.048699340D+01	-5.910641150D-04	1.301993020D-07				
-1.490682940D-11	6.903573410D-16		-1.306290160D+05	-8.031642952D+01				

P3 Gurvich,1989 pt1 p402 pt2 p256.

2 tpris89 P	3.00	0.00	0.00	0.00	0.00	0	92.9212830	210000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.693358950D+04	-8.643589320D+02	8.734247530D+00	1.094534560D-05	-1.998573320D-06				
2.096750510D-09	-6.922889710D-13		2.774847340D+04	-2.063587261D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.253513060D+05	-8.306734620D+01	7.561956770D+00	-2.474403950D-05	5.457276930D-09				
-6.244660570D-13	2.887724220D-17		2.308722280D+04	-1.228310621D+01				

P3O6 Gurvich,1989 pt1 p412 pt2 p265.

2 tpris89 P	3.000	6.00	0.00	0.00	0.00	0	188.9176830	-1575681.029
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.014493813D+05	-3.053488073D+03	1.602114098D+01	4.316889900D-02	-6.376544260D-05				
4.422867920D-08	-1.200020334D-11		-1.776503811D+05	-6.556267890D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.787968100D+05	-1.651988071D+03	2.772258397D+01	-4.859326700D-04	1.067867708D-07				
-1.218015776D-11	5.614911960D-16		-1.909165548D+05	-1.220665277D+02				

## Appendix D (continued)

P4 Gurvich,1989 pt1 p402 pt2 p257.

2 tps89 P	4.00	0.00	0.00	0.00	0.00	0.00	0	123.8950440	58900.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.205141850D+05	-2.345711790D+03	1.773946550D+01	-1.456314970D-02	1.587594090D-05					
-9.314710310D-09	2.271491670D-12		1.608846480D+04	-7.088590647D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.858705860D+05	-6.284546890D+01	1.004844880D+01	-1.987668850D-05	4.482408440D-09					
-5.226103670D-13	2.455791290D-17		3.848210920D+03	-2.477297797D+01					

P406 Gurvich,1989 pt1 p413 pt2 p266.

2 tps89 P	4.000	6.00	0.00	0.00	0.00	0	219.8914440	-1606000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.760894750D+05	-5.685832620D+03	2.914225450D+01	2.251532120D-02	-4.510269630D-05				
3.588312690D-08	-1.057572060D-11		-1.688562480D+05	-1.451359851D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.008997240D+06	-8.872753990D+02	2.866064830D+01	-2.636018940D-04	5.810940720D-08				
-6.648086960D-12	3.074391930D-16		-1.997138900D+05	-1.281853821D+02				

P407 Gurvich,1989 pt1 p414 pt2 p267.

2 tps89 P	4.000	7.00	0.00	0.00	0.00	0	235.8908440	-1984448.045
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.218586960D+05	-4.871444730D+03	2.454417068D+01	4.015509550D-02	-6.524197150D-05				
4.756554180D-08	-1.332975491D-11		-2.184517427D+05	-1.181504792D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.102947375D+06	-1.511077128D+03	3.210979500D+01	-4.371803760D-04	9.516639610D-08				
-1.075204176D-11	4.911025680D-16		-2.429096540D+05	-1.473140859D+02				

P408 Gurvich,1989 pt1 p415 pt2 p268.

2 tps89 P	4.000	8.00	0.00	0.00	0.00	0	251.8902440	-2302214.078
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.719326942D+05	-4.118600390D+03	2.028714235D+01	5.685416990D-02	-8.400739630D-05				
5.823389060D-08	-1.578647160D-11		-2.604539703D+05	-9.407162070D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.173177311D+06	-2.200632995D+03	3.563010130D+01	-6.489849740D-04	1.429623989D-07				
-1.635821725D-11	7.571070760D-16		-2.783843144D+05	-1.679636960D+02				

P409 Gurvich,1989 pt1 p416 pt2 p269.

2 tps89 P	4.000	9.00	0.00	0.00	0.00	0	267.8896440	-2613979.111
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.199916395D+05	-3.336464940D+03	1.586413106D+01	7.402452330D-02	-1.034835052D-04				
6.944438320D-08	-1.840733450D-11		-3.018742692D+05	-6.997967670D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.233696783D+06	-2.917032808D+03	3.917757110D+01	-8.736402980D-04	1.937914895D-07				
-2.230510118D-11	1.037248818D-15		-3.129637516D+05	-1.897176420D+02				

P4010 Gurvich,1989 pt1 p419 pt2 p271.

2 tps89 P	4.000	10.00	0.00	0.00	0.00	0	283.8890440	-2906223.447
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.670142268D+05	-2.540243300D+03	1.136853403D+01	9.137812160D-02	-1.231990626D-04				
8.081032230D-08	-2.106787011D-11		-3.410151910D+05	-4.643431340D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.337201132D+06	-3.516382330D+03	4.260403310D+01	-1.037406404D-03	2.287613089D-07				
-2.620219946D-11	1.213529528D-15		-3.459515050D+05	-2.115498906D+02				

Pb Hf:Gurvich,1991. Moore,1971. Moore,1970a. Gordon,1999.

3 g 8/97 PB	1.00	0.00	0.00	0.00	0.00	0	207.2000000	195200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.213382285D+03	-1.906116019D+01	2.619299546D+00	-3.829519610D-04	6.688180450D-07				
-6.061231080D-10	2.240022429D-13		2.282096238D+04	6.201369200D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.084313070D+06	2.672673180D+04	-2.626244039D+01	1.358282305D-02	-2.685523566D-06				
2.352432800D-10	7.324114532D-15		-1.481650666D+05	2.154011624D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.325474970D+08	-2.751419152D+05	6.303031930D+01	-6.813672740D-03	4.447489610D-07				
-1.519361678D-11	2.043475665D-16		2.243651683D+06	-5.225649900D+02				

Pb+ Moore1971. Moore,1970a. Gordon,1999.

3 g10/97 PB	1.00E	-1.00	0.00	0.00	0.00	0	207.1994514	916996.528
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.486689040D+00	-1.134955793D-01	2.500549799D+00	-1.382464681D-06	1.906022991D-09				
-1.368396828D-12	4.003528117D-16		1.095438901D+05	7.538855900D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.320690183D+06	-4.096048010D+03	7.389101510D+00	-2.807751909D-03	7.830991650D-07				
-9.310600910D-11	4.016371727D-15		1.354347306D+05	-2.722020908D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.101539500D+08	-2.538072503D+05	6.239804790D+01	-6.542962120D-03	3.507316530D-07				
-8.114133770D-12	5.908352630D-17		2.122867468D+06	-5.163550210D+02				

## Appendix D (continued)

Pb- Hotop,1985. Gordon,1999.

3 g 9/97 PB	1.00E	1.00	0.00	0.00	0.00	0	207.2005486	153881.928
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						1.776226140D+04	8.235132100D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						1.776226140D+04	8.235132100D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						1.776226140D+04	8.235132100D+00

PbBr Gurvich,1991 pt1 p434 pt2 p360.

2 tpis91 PB	1.00BR	1.00	0.00	0.00	0.00	0	287.1040000	64821.322
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.393487988D+03	-4.576591210D+01	4.692608280D+00	-3.845290630D-04	5.888213500D-07				
-4.084792890D-10	1.202515201D-13		6.662434770D+03	5.991705510D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.581831670D+06	7.143490760D+03	-2.658193640D+00	3.107722260D-03	-4.631381540D-07				
1.095529211D-11	1.508555088D-15		-3.970440980D+04	5.959238650D+01				

PbBr2 Gurvich,1991 pt1 p437 pt2 p362.

2 tpis91 PB	1.00BR	2.00	0.00	0.00	0.00	0	367.0080000	-103908.063
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.172766360D+03	-6.783207630D+01	7.273156140D+00	-5.990596120D-04	7.358634610D-07				
-4.743604810D-10	1.246922291D-13		-1.427890796D+04	-6.987992150D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.320421479D+04	-1.143074947D+00	7.000972540D+00	-4.284471610D-07	1.018044861D-10				
-1.234016791D-14	5.971337650D-19		-1.462213750D+04	8.868582650D-01				

PbBr3 Gurvich,1991 pt1 p438 pt2 p363.

2 tpis91 PB	1.00BR	3.00	0.00	0.00	0.00	0	446.9120000	-104010.957
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.164424250D+04	-1.555151665D+02	1.062317321D+01	-1.361947117D-03	1.668738791D-06				
-1.073686019D-09	2.818250340D-13		-1.478208304D+04	-1.443758579D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.787930766D+04	-2.633265111D+00	1.000223199D+01	-9.807761410D-07	2.326232632D-10				
-2.815994460D-14	1.361283735D-18		-1.556981182D+04	-1.081765474D+01				

PbBr4 Gurvich,1991 pt1 p439 pt2 p364.

2 tpis91 PB	1.00BR	4.00	0.00	0.00	0.00	0	526.8160000	-182435.511
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.176458199D+04	-2.567166983D+02	1.402223292D+01	-2.224117068D-03	2.716201994D-06				
-1.743340164D-09	4.567359750D-13		-2.462125551D+04	-2.882020750D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.880216030D+04	-4.382933770D+00	1.300369823D+01	-1.620061335D-06	3.834130880D-10				
-4.633967180D-14	2.237427066D-18		-2.592327065D+04	-2.287710636D+01				

PbCL Gurvich,1991 pt1 p427 pt2 p355.

2 tpis91 PB	1.00CL	1.00	0.00	0.00	0.00	0	242.6530000	8819.118
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.902700749D+03	-8.293459710D+01	4.714824480D+00	-1.931473228D-04	9.105579020D-08				
5.419385230D-11	3.284969700D-14		1.254460217D+02	4.323194455D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.854285530D+05	6.922197500D+02	4.509971240D+00	-6.853421300D-04	5.087395500D-07				
-9.772753810D-11	5.807471580D-15		-5.269684720D+03	6.646491015D+00				

PbCL2 Gurvich,1991 pt1 p430 pt2 p357.

2 tpis91 PB	1.00CL	2.00	0.00	0.00	0.00	0	278.1060000	-175547.471
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.830580143D+03	-3.134256659D+02	8.212827290D+00	-2.585096173D-03	3.109456077D-06				
-1.972978208D-09	5.123542480D-13		-2.167569042D+04	-9.219412244D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.149192744D+04	-5.565477580D+00	7.004599540D+00	-1.986025455D-06	4.651719590D-10				
-5.579137010D-14	2.678143570D-18		-2.327439309D+04	-2.140739285D+00				

PbCL3 Gurvich,1991 pt1 p432 pt2 p358.

2 tpis91 PB	1.00CL	3.00	0.00	0.00	0.00	0	313.5590000	-177653.507
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.623588970D+02	-5.253152750D+02	1.203336337D+01	-4.335184980D-03	5.215698350D-06				
-3.310022380D-09	8.596970610D-13		-2.180576379D+04	-2.694206962D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.664412790D+04	-9.329514790D+00	1.000771099D+01	-3.329727570D-06	7.799330810D-10				
-9.354606100D-14	4.490589700D-18		-2.448508643D+04	-1.507490870D+01				

## Appendix D (continued)

PbCL4 Gurvich,1991 pt1 p433 pt2 p359.  
 2 tps91 PB 1.00CL 4.00 0.00 0.00 0.00 0 349.0120000 -327430.362  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23449.438  
 1.739405796D+04-8.902139320D+02 1.637565058D+01-7.088992260D-03 8.432567340D-06  
 -5.305309390D-09 1.368671294D-12 -3.888215620D+04-4.850133784D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23449.438  
 -8.266679560D+04-1.639486405D+01 1.301336711D+01-5.716141400D-06 1.329368390D-09  
 -1.585922492D-13 7.581763610D-18 -4.343984220D+04-2.874559263D+01

PbF Gurvich,1991 pt1 p419 pt2 p350.  
 2 tps91 PB 1.00F 1.00 0.00 0.00 0.00 0 226.1984032 -98867.789  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9268.111  
 2.684864255D+04-4.751725640D+02 6.019644370D+00-2.718531008D-03 2.942882954D-06  
 -1.687543009D-09 4.086122080D-13 -1.079038653D+04-4.983048840D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9268.111  
 -4.734202750D+05 1.027785283D+03 3.888658730D+00-1.649813448D-04 2.931163260D-07  
 -5.766459650D-11 3.247486190D-15 -2.026165076D+04 9.319483890D+00

PbF2 Gurvich,1991 pt1 p424 pt2 p352.  
 2 tps91 PB 1.00F 2.00 0.00 0.00 0.00 0 245.1968064 -443427.390  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12572.610  
 5.920552280D+04-1.052529292D+03 1.028969284D+01-5.876346270D-03 6.102333130D-06  
 -3.424792640D-09 8.024025420D-13 -4.999050000D+04-2.525115478D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12572.610  
 -8.505899770D+04-3.074244334D+01 7.023346040D+00-9.455183590D-06 2.108489027D-09  
 -2.434212002D-13 1.133872429D-17 -5.552236770D+04-5.496073220D+00

PbF3 Gurvich,1991 pt1 p425 pt2 p353.  
 2 tps91 PB 1.00F 3.00 0.00 0.00 0.00 0 264.1952096 -489572.613  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15535.047  
 8.55309870D+04-1.731036694D+03 1.556596150D+01-1.022225919D-02 1.089984998D-05  
 -6.269998820D-09 1.502616508D-12 -5.300335670D+04-5.335733480D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15535.047  
 -1.459704258D+05-4.820396430D+01 1.003685845D+01-1.501095764D-05 3.362474990D-09  
 -3.896020710D-13 1.820152103D-17 -6.206869590D+04-2.006978661D+01

PbF4 Gurvich,1991 pt1 p426 pt2 p354.  
 2 tps91 PB 1.00F 4.00 0.00 0.00 0.00 0 283.1936128 -799925.173  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19626.227  
 1.309963563D+05-2.307299499D+03 1.945201440D+01-1.024522729D-02 9.395874960D-06  
 -4.626894150D-09 9.450881430D-13 -8.804147460D+04-7.524645820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19626.227  
 -2.132616322D+05-8.578621950D+01 1.306428551D+01-2.575563598D-05 5.693324590D-09  
 -6.526219550D-13 3.022341960D-17 -1.002908979D+05-3.590240280D+01

PbI Gurvich,1991 pt1 p440 pt2 p365.  
 2 tps91 PB 1.00I 1.00 0.00 0.00 0.00 0 334.1044700 108904.324  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10339.124  
 -2.717334060D+03-1.542541996D+01 4.565327900D+00-1.061215818D-04 2.414841342D-07  
 -1.876070301D-10 6.460614270D-14 1.181864978D+04 7.669802670D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10339.124  
 -3.901070250D+06 1.147976718D+04-8.176109020D+00 6.523454700D-03-1.522611682D-06  
 1.626692202D-10-6.553328880D-15 -6.154433690D+04 9.938404970D+01

PbI2 Gurvich,1991 pt1 p443 pt2 p367.  
 2 tps91 PB 1.00I 2.00 0.00 0.00 0.00 0 461.0089400 -10252.630  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15247.370  
 -5.904986720D+03-4.833307030D+01 7.195438030D+00-4.298600090D-04 5.291412070D-07  
 -3.416402820D-10 8.991341920D-14 -3.107780155D+03 1.324773678D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15247.370  
 -1.088339477D+04-8.164418370D-01 7.000697300D+00-3.079876763D-07 7.331718140D-11  
 -8.899193880D-15 4.310712500D-19 -3.352096380D+03 2.458605463D+00

PbI3 Gurvich,1991 pt1 p444 pt2 p368.  
 2 tps91 PB 1.00I 3.00 0.00 0.00 0.00 0 587.9134100 21755.412  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21065.012  
 -1.014996331D+04-5.938078200D+01 1.024073798D+01-5.304694530D-04 6.538623030D-07  
 -4.225895720D-10 1.113029818D-13 -1.138482403D+02-8.975540500D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21065.012  
 -1.624229573D+04-1.002945584D+00 1.000085839D+01-3.796679740D-07 9.046751720D-11  
 -1.098840054D-14 5.325388290D-19 -4.138258930D+02-7.579417110D+00

## Appendix D (continued)

PbI4 Gurvich,1991 pt1 p445 pt2 p369.

2 tps91 PB	1.00I	4.00	0.00	0.00	0.00	0.00	0	714.8178800	-41226.459
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.217096972D+04	-7.226317440D+01	1.329294204D+01	-6.454660900D-04	7.955761850D-07					
-5.141632830D-10	1.354188031D-13		-8.528148680D+03	-2.010457498D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.958477744D+04	-1.223385179D+00	1.300104732D+01	-4.633295690D-07	1.104213978D-10					
-1.341397771D-14	6.501706110D-19		-8.893193200D+03	-1.840570345D+01					

PbO Gurvich,1991 pt1 p413 pt2 p345.

2 tps91 PB	1.00O	1.00	0.00	0.00	0.00	0	223.1994000	68137.108	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.424025000D+04	-4.198050110D+02	4.720306410D+00	1.451061751D-03	-3.206035460D-06					
2.713956273D-09	-8.333275610D-13		9.253186470D+03	4.482891210D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.426996850D+05	-1.107731354D+02	3.180684490D+00	1.991815065D-03	-1.079782025D-06					
2.540990941D-10	-1.834652493D-14		8.339391540D+03	1.050920926D+01					

PbO2 Gurvich,1991 pt1 p416 pt2 p347.

2 tps91 PB	1.00O	2.00	0.00	0.00	0.00	0	239.1988000	136152.734	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.071058290D+04	-1.076757462D+03	9.401711730D+00	-1.003861584D-03	-1.233815617D-06					
1.858386979D-09	-6.834621210D-13		1.999645981D+04	-2.503976748D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.307796670D+05	-7.314361450D+01	7.554083410D+00	-2.143421561D-05	4.696464000D-09					
-5.344972180D-13	2.460760535D-17		1.413386101D+04	-1.252684909D+01					

PbS Gurvich,1991 pt1 p448 pt2 p371.

2 tps91 PB	1.00S	1.00	0.00	0.00	0.00	0	239.2650000	127945.313	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.529840503D+04	-3.439746350D+02	5.680630640D+00	-2.232931917D-03	2.504608209D-06					
-1.470427328D-09	3.577527190D-13		1.578551202D+04	-2.628900926D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.105441649D+06	-5.520413580D+03	9.369249260D+00	-1.410262019D-03	-1.642683362D-07					
1.451447577D-10	-1.393564925D-14		5.009334530D+04	-3.217417657D+01					

PbS2 Gurvich,1991 pt1 p450 pt2 p372.

2 tps91 PB	1.00S	2.00	0.00	0.00	0.00	0	271.3300000	244049.005	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.446375880D+04	-6.654855460D+02	9.920201180D+00	-4.924194380D-03	5.716906290D-06					
-3.529488830D-09	8.971138350D-13		3.044310130D+04	-2.295765552D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.416700300D+04	-1.343600342D+01	7.510700360D+00	-4.497318630D-06	1.032444494D-09					
-1.219580043D-13	5.785804650D-18		2.701229533D+04	-8.714618097D+00					

Rb Hf:Cox,1989. Moore,1971. Moore,1970a. Gordon,1999.

3 g 1/98 RB	1.00	0.00	0.00	0.00	0.00	0	85.4678000	80900.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.352856616D+01	-2.042232679D-01	2.501213823D+00	-3.650619900D-06	5.884722670D-09					
-4.842274720D-12	1.596211946D-15		8.985569210D+03	6.207005480D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.138274064D+06	3.804041940D+03	-2.750899258D+00	3.891460700D-03	-1.632296823D-06					
3.511893140D-10	-2.521064422D-14		-1.466454849D+04	4.253442370D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.245192200D+08	-3.493850870D+05	1.159097652D+02	-1.492843123D-02	9.582385060D-07					
-2.996233671D-11	3.657332046D-16		2.636178014D+06	-9.586517230D+02					

Rb+ Moore,1971. IP:Moore,1970a. Gordon,1999.

3 g 1/98 RB	1.00E	-1.00	0.00	0.00	0.00	0	85.4672514	490129.128	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		5.820327360D+04	5.520506920D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		5.820327360D+04	5.520506920D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.120352830D+07	-2.920376515D+04	1.102096776D+01	-1.311457972D-03	1.124752629D-07					
-5.107819770D-12	9.622794537D-17		2.850166118D+05	-6.672202250D+01					

## Appendix D (continued)

Rb- Hotop,1985. Gordon,1999.

3 g 9/97 RB	1.00E	1.00	0.00	0.00	0.00	0.00	0.00	85.4683486	27818.528
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						2.600405796D+03	5.520526170D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						2.600405796D+03	5.520526170D+00	
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
0.000000000D+00	0.000000000D+00						2.600405796D+03	5.520526170D+00	

RbBO2 Gurvich,1982 pt1 p459 pt2 p483.

2 tpis82 RB	1.00B	1.000	2.00	0.00	0.00	0.00	0.00	128.2776000	-678977.302
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.198657750D+04	-6.799448330D+02	8.185151010D+00	2.772536733D-03	-6.175770470D-07					
-9.426136250D-10	4.722414240D-13						-8.020339590D+04	-1.239198887D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.154463400D+04	-1.668328341D+03	1.117268757D+01	-4.505533530D-04	9.681330590D-08					
-1.088037652D-11	4.967733660D-16						-7.507903250D+04	-3.131951149D+01	

RbBr Gurvich,1982 pt1 p446 pt2 p470.

2 tpis82 RB	1.00BR	1.00	0.00	0.00	0.00	0.00	0.00	165.3718000	-191510.876
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.703859700D+03	2.092281597D+01	4.370607370D+00	4.494604780D-04	-4.835438840D-07					
3.526068600D-10	9.886538320D-14						-2.449112515D+04	6.427431700D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.609092474D+06	-4.466774590D+03	9.064092060D+00	-1.995333358D-03	4.016633520D-07					
-4.163091400D-12	-3.092443341D-15						4.427467690D+03	-2.757714089D+01	

RbCL Gurvich,1982 pt1 p443 pt2 p467.

2 tpis82 RB	1.00CL	1.00	0.00	0.00	0.00	0.00	0.00	120.9208000	-223322.879
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.740809580D+03	-1.528835285D+01	4.515200900D+00	1.067270745D-04	-6.385945590D-09					
-1.301381692D-11	1.641459742D-14						-2.814243986D+04	4.190115141D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.143043004D+06	4.003861880D+03	-1.096156782D+00	4.033581280D-03	-1.454151464D-06					
-2.719263762D-10	-1.810463980D-14						-5.297686040D+04	4.311317822D+01	

RbF Gurvich,1982 pt1 p440 pt2 p464.

2 tpis82 RB	1.00F	1.00	0.00	0.00	0.00	0.00	0.00	104.4662032	-333511.885
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.287360190D+04	-6.080907460D+02	7.406622360D+00	-7.277864720D-03	1.013930727D-05					
-7.141372500D-09	2.014332982D-12						-3.849834130D+04	-1.375750778D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.544811150D+05	2.633756505D+03	1.216216506D+00	2.136494067D-03	-6.728426080D-07					
1.134905135D-10	-6.825624440D-15						-5.810179110D+04	2.588118896D+01	

RbH Gurvich,1982 pt1 p435 pt2 p459.

2 tpis82 RB	1.00H	1.00	0.00	0.00	0.00	0.00	0.00	86.4757400	119324.106
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.908270610D+03	4.649870400D+01	1.833967623D+00	8.444279140D-03	-1.167538647D-05					
8.010389420D-09	-2.162578321D-12						1.328248009D+04	1.279544976D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.937703530D+06	9.379817260D+03	-7.542563460D+00	7.493226800D-03	-2.159228887D-06					
2.871300173D-10	-1.459981256D-14						-4.595518830D+04	8.365664320D+01	

RbI Gurvich,1982 pt1 p449 pt2 p473.

2 tpis82 RB	1.00I	1.00	0.00	0.00	0.00	0.00	0.00	212.3722700	-138480.874
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.693052800D+02	-2.968608844D+01	4.648745840D+00	-2.962415236D-04	5.978135340D-07					
-4.351255250D-10	1.313617336D-13						-1.786610717D+04	5.812409830D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.297424850D+06	-1.296911161D+04	1.958730402D+01	-8.458425590D-03	2.463480035D-06					
-3.191575730D-10	1.458455589D-14						6.432948040D+04	-1.009499336D+02	

RbK Gurvich,1982 pt1 p462 pt2 p486.

2 tpis82 RB	1.00K	1.00	0.00	0.00	0.00	0.00	0.00	124.5661000	120013.330
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.494695429D+04	-4.553060660D+02	7.686189950D+00	-1.108112244D-02	2.093398586D-05					
-1.824445366D-08	5.617645360D-12						1.516136160D+04	-1.063563675D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.175391070D+06	5.918588510D+03	9.202649420D+00	-1.060933600D-02	4.964826060D-06					
-8.716698790D-10	5.221887960D-14						-3.272769040D+04	-1.372401997D+01	



## Appendix D (continued)

RbLi Gurvich,1982 pt1 p460 pt2 p484.

2 tpis82 RB	1.00LI	1.00	0.00	0.00	0.00	0.00	0	92.4088000	164181.324
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.263413044D+03	-2.888496910D+01	4.555826540D+00	3.625667530D-04	-9.598002220D-07					
1.631010244D-09	-8.159825980D-13		1.853455250D+04	2.831743182D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.085515194D+07	-3.805106970D+04	5.516555040D+01	-3.128845612D-02	9.261650250D-06					
-1.264671408D-09	6.431662050D-14		2.543964131D+05	-3.520758710D+02					

RbNO2 Gurvich,1982 pt1 p454 pt2 p478.

2 tpis82 RB	1.00N	1.000	2.00	0.00	0.00	0	131.4733000	-187629.777	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.199420030D+04	1.265802595D+03	-2.415715742D+00	3.054641420D-02	-3.684004050D-05					
2.247716481D-08	-5.547527430D-12		-3.037381667D+04	4.814256904D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.644994453D+05	-8.499443440D+02	1.063080575D+01	-2.517893988D-04	5.561420120D-08					
-6.378805600D-12	2.957679896D-16		-2.128590982D+04	-2.568367325D+01					

RbNO3 Gurvich,1982 pt1 p456 pt2 p480.

2 tpis82 RB	1.00N	1.000	3.00	0.00	0.00	0	147.4727000	-314972.483	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.664669172D+04	8.807634790D+02	-3.159459457D+00	4.271229020D-02	-5.351029210D-05					
3.360969750D-08	-8.503290510D-12		-4.353595460D+04	4.943052899D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.147413867D+05	-1.371457846D+03	1.401319759D+01	-4.030275020D-04	8.878332290D-08					
-1.016221214D-11	4.704254090D-16		-3.504339940D+04	-4.619379241D+01					

RbNa Gurvich,1982 pt1 p461 pt2 p485.

2 tpis82 RB	1.00NA	1.00	0.00	0.00	0.00	0	108.4575700	131470.328	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.974455567D+04	-5.082790590D+02	7.734033520D+00	-1.013006840D-02	1.745455325D-05					
-1.398725470D-08	3.968106770D-12		1.682379436D+04	-1.240085290D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.297114270D+06	-1.831013588D+04	3.454394200D+01	-2.230134993D-02	7.339874530D-06					
-1.064784996D-09	5.617598460D-14		1.242610951D+05	-1.993661980D+02					

RbO Gurvich,1982 pt1 p429 pt2 p452.

2 tpis82 RB	1.00O	1.00	0.00	0.00	0.00	0	101.4672000	52489.324	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.900081316D+05	-3.428228990D+03	2.480251273D+01	-5.051654580D-02	6.476338760D-05					
-4.198012420D-08	1.093889043D-11		2.083898450D+04	-1.097559150D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.170756880D+05	-2.175089620D+03	8.290412210D+00	-2.996487663D-03	1.233144275D-06					
-2.115810631D-10	1.242607430D-14		1.828164827D+04	-2.117386042D+01					

RbOH Gurvich,1997.

2 g 9/97 RB	1.00O	1.00H	1.00	0.00	0.00	0	102.4751400	-238000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.213832721D+04	-5.441411590D+02	8.459814640D+00	-3.561526560D-03	2.992872390D-06					
-7.280267400D-10	-4.553847180D-14		-2.787262486D+04	-1.913421991D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.958583130D+05	-2.332339000D+03	7.971192480D+00	1.044439355D-04	-6.328257750D-08					
1.029358824D-11	-5.743277790D-16		-1.515568947D+04	-1.950051629D+01					

Rb2Br2 Gurvich,1982 pt1 p447 pt2 p471.

2 tpis82 RB	2.00BR	2.00	0.00	0.00	0.00	0	330.7436000	-551801.433	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.005525400D+03	-2.111968088D+01	1.008629404D+01	-1.911936090D-04	2.366059490D-07					
-1.533722380D-10	4.048725060D-14		-6.927313600D+04	-9.622434630D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.014535336D+04	-3.601550320D-01	1.000031058D+01	-1.380745805D-07	3.302067950D-11					
-4.021581820D-15	1.953006729D-19		-6.937960880D+04	-9.122562360D+00					

Rb2CL2 Gurvich,1982 pt1 p444 pt2 p468.

2 tpis82 RB	2.00CL	2.00	0.00	0.00	0.00	0	241.8416000	-618373.536	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.125039522D+04	-6.756953990D+01	1.027381915D+01	-6.031848990D-04	7.433324780D-07					
-4.803372160D-10	1.264973638D-13		-7.706757500D+04	-1.363652575D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.818875133D+04	-1.137903580D+00	1.000097318D+01	-4.302156400D-07	1.024725787D-10					
-1.244291058D-14	6.028912390D-19		-7.740897670D+04	-1.204843385D+01					

## Appendix D (continued)

Rb2F2                      Gurvich,1982 pt1 p441 pt2 p465.

2	tpis82 RB	2.00F	2.00	0.00	0.00	0.00	0	208.9324064	-854913.348
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-8.178347100D+03	-3.334733540D+02	1.131540799D+01	-2.842914926D-03	3.454959580D-06					
-2.209373419D-09	5.772073270D-13		-1.042230504D+05	-2.368991587D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.376574390D+04	-5.761452040D+00	1.000482691D+01	-2.104159548D-06	4.962416270D-10					
-5.982174970D-14	2.882751742D-18		-1.059176154D+05	-1.603254014D+01					

Rb2I2                      Gurvich,1982 pt1 p450 pt2 p474.

2	tpis82 RB	2.00I	2.00	0.00	0.00	0.00	0	424.7445400	-432956.482
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.839663550D+03	-9.527537900D+00	1.003904495D+01	-8.668754000D-05	1.074384368D-07					
-6.972122230D-11	1.842065721D-14		-5.502780960D+04	-7.174113320D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.799834640D+03	-1.642527699D-01	1.000014200D+01	-6.321420730D-08	1.512811170D-11					
-1.843027189D-15	8.951244180D-20		-5.507579620D+04	-6.948045390D+00					

Rb2O                      Gurvich,1982 pt1 p431 pt2 p455.

2	tpis82 RB	2.00O	1.00	0.00	0.00	0.00	0	186.9350000	-108929.421
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.971276138D+04	-4.627508860D+02	8.588293130D+00	-3.085559728D-03	3.451980140D-06					
-2.068570368D-09	5.132480500D-13		-1.284854711D+04	-1.264891828D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.846360090D+04	-1.082831019D+01	7.008421890D+00	-3.476228120D-06	7.869785060D-10					
-9.195683850D-14	4.325201520D-18		-1.525373768D+04	-3.230388780D+00					

Rb2O2                      Gurvich,1982 pt1 p434 pt2 p457.

2	tpis82 RB	2.00O	2.00	0.00	0.00	0.00	0	202.9344000	-215848.468
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.260553230D+04	-7.578164720D+02	1.070815124D+01	1.148004329D-03	-3.291243670D-06					
2.853106637D-09	-8.721590680D-13		-2.475317258D+04	-2.434276460D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.318567396D+05	-9.647737790D+01	1.007222726D+01	-2.894921706D-05	6.405639100D-09					
-7.351419390D-13	3.408561710D-17		-2.882179733D+04	-1.910948823D+01					

Rb2O2H2                      Gurvich,1997. .

2	g 9/97 RB	2.00O	2.00H	2.00	0.00	0.00	0	204.9502800	-639000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.577076530D+03	-8.417631000D+02	1.704083828D+01	-5.357882540D-03	3.951778770D-06					
-2.051775094D-10	-4.085416910D-13		-7.694982170D+04	-5.435412780D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.792711652D+06	-4.659406600D+03	1.693822422D+01	2.106246492D-04	-1.269617470D-07					
2.063382927D-11	-1.150861507D-15		-5.024117630D+04	-6.027054920D+01					

Rb2SO4                      Gurvich,1982 pt1 p452 pt2 p476.

2	g10/99 RB	2.00S	1.00O	4.00	0.00	0.00	0	266.9982000	-1096592.052
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.094854930D+04	-6.889705900D+02	7.034242180D+00	3.933945470D-02	-5.498920510D-05					
3.716341080D-08	-9.919863380D-12		-1.311877657D+05	-4.450168488D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.302898310D+05	-9.515435450D+02	1.971013517D+01	-2.842916301D-04	6.289142940D-08					
-7.219324300D-12	3.348718190D-16		-1.338713151D+05	-7.056246882D+01					

Rn                      Ref-Elm. Moore,1971. Gordon,1999.

3	g 5/97 RN	1.00	0.00	0.00	0.00	0.00	0	222.0176000	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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
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
9.180866680D+08	-6.245854600D+05	1.724946531D+02	-2.325758595D-02	1.636222413D-06					
-5.369173150D-11	6.507189926D-16		4.883105900D+06	-1.449516146D+03					

Rn+                      Moore,1971. Gordon,1999.

3	g 1/97 RN	1.00E	-1.00	0.00	0.00	0.00	0	222.0170514	1043270.264
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.697148970D-02	1.106742047D-03	2.499994937D+00	1.189388239D-08	-1.515895754D-11					
9.958934810D-15	-2.640751817D-18		1.247304760D+05	8.338761700D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.998285319D+04	5.930675660D+01	2.432476003D+00	3.716025920D-05	-1.012057848D-08					
1.192256661D-12	-3.184521980D-17		1.243528478D+05	8.821997790D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.408821471D+07	1.571151698D+04	-1.411683762D+00	4.495267600D-04	-2.324033616D-08					
5.830243350D-13	-5.821682810D-18		9.187457500D+02	4.233613280D+01					

## Appendix D (continued)

Hf: Cox,1989 p22. Martin,1990. Gordon,1999.									
3 g 5/97 S	1.00	0.00	0.00	0.00	0.00	0	32.0650000	277170.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.174841820D+02	-1.924704923D+02	4.686825930D+00	-5.841365600D-03	7.53853520D-06					
-4.863586040D-09	1.256976992D-12						3.323592180D+04	-5.718523969D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.854244790D+05	1.438830408D+03	1.258504116D+00	3.797990430D-04	1.630685864D-09					
-9.547095850D-12	8.041466646D-16						2.334995270D+04	1.559554855D+01	
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.302005414D+08	6.909362020D+04	-1.176228025D+01	1.601540850D-03	-1.050533340D-07					
4.341829020D-12	-7.675621927D-17						-5.261485030D+05	1.322195251D+02	
S+ Martin,1990. Gordon,1999.									
3 g 1/98 S	1.00E	-1.00	0.00	0.00	0.00	0	32.0644514	1282496.428	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00						1.535026117D+05	5.436223340D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.346218684D+06	-4.056871510D+03	7.153436550D+00	-2.523562352D-03	6.429539610D-07					
-6.431672160D-11	2.141387919D-15						1.792823835D+05	-2.786935079D+01	
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.542254583D+08	-1.023073546D+05	2.591796942D+01	-2.111469141D-03	9.215571560D-08					
-1.964168821D-12	2.096218597D-17						9.622418410D+05	-2.017239957D+02	
S- Hotop,1985. Gordon,1999.									
3 g 4/97 S	1.00E	1.00	0.00	0.00	0.00	0	32.0655486	70368.505	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.596051473D+03	-1.422398653D+02	4.007825670D+00	-3.608855910D-03	4.236230000D-06					
-2.520987604D-09	6.079479760D-13						8.197793070D+03	-2.582377345D+00	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.730311692D+03	1.414072078D+02	2.403340775D+00	3.693577530D-05	-7.944080440D-09					
8.952208380D-13	-4.099662820D-17						6.931195700D+03	6.574986902D+00	
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.223682088D+05	1.203125842D+02	2.473942293D+00	2.935459895D-06	-1.808577869D-10					
5.778854260D-15	-7.490337240D-20						6.947841220D+03	6.070579772D+00	
SCL Chase,1998 p803.									
2 j 6/78 S	1.00CL	1.00	0.00	0.00	0.00	0	67.5180000	156465.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.613051454D+04	-5.606249550D+02	8.064931130D+00	-9.186326400D-03	1.224205395D-05					
-8.209562020D-09	2.205087197D-12						1.997739280D+04	-1.693354410D+01	
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.405123450D+04	3.629760850D+02	4.069959360D+00	3.034029742D-04	-8.248301390D-08					
1.252700734D-11	-6.417463650D-16						1.523111069		

## Appendix D (continued)

SF Gurvich,1989 pt1 p302 pt2 p183.

2	tpis89 S	1.00F	1.00	0.00	0.00	0.00	0	51.0634032	15445.561
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.206456774D+04	-2.910270770D+02	5.480101570D+00	-1.975880235D-03	2.473685990D-06					
-1.610904623D-09	4.310038540D-13			1.991337574D+03	-4.544138975D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.634580750D+05	-2.423638430D+03	7.352198710D+00	-1.598026079D-03	4.868515020D-07					
-6.478000530D-11	2.980297310D-15			1.577461591D+04	-1.902584835D+01				

SF+ Chase,1998 p1091 6/76.

3	g 1/01 S	1.00F	1.00E	-1.00	0.00	0.00	0	51.0628546	994570.218
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.578303670D+04	-6.986699970D+02	5.621292240D+00	-6.909274110D-04	-1.282392780D-07					
4.021320420D-10	-1.424033453D-13			1.221751247D+05	-6.682377715D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.374943900D+05	2.377214240D+03	2.052929113D+00	1.081609837D-03	-1.535468024D-07					
8.222691900D-12	3.259746880D-17			1.026849122D+05	1.887705768D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.833080340D+07	3.315103280D+04	-4.246678200D+00	1.269355284D-03	-7.864010490D-08					
-2.406680266D-12	-2.892795916D-17			-1.419262455D+05	7.611520762D+01				

SF- Gurvich,1989 pt1 p304 pt2 p184.

2	tpis89 S	1.00F	1.00E	1.00	0.00	0.00	0	51.0639518	-231346.893
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.019879280D+04	-5.321549310D+02	4.904849010D+00	9.915307420D-04	-2.270841545D-06					
1.844749756D-09	-5.357057200D-13			-2.611388646D+04	-3.637468065D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.068923125D+05	-1.324372811D+03	6.646211240D+00	-1.641781588D-03	6.783883120D-07					
-1.198331099D-10	7.121739540D-15			-2.150994816D+04	-1.470239183D+01				

SF2 Gurvich,1989 pt1 p305 pt2 p185.

2	tpis89 S	1.00F	2.00	0.00	0.00	0.00	0	70.0618064	-293188.734
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.870871130D+04	-8.432418250D+02	6.269496400D+00	6.484142450D-03	-1.145126533D-05					
8.770291560D-09	-2.542611601D-12			-3.229980700D+04	-8.800025780D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.702612287D+05	-1.497038204D+02	7.110934140D+00	-4.407741600D-05	9.682208310D-09					
-1.104468959D-12	5.095308780D-17			-3.704289490D+04	-1.095253960D+01				

SF2+ Chase,1998 p1144 12/76.

3	g 1/01 S	1.00F	2.00E	-1.00	0.00	0.00	0	70.0612578	706015.901
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.311648923D+05	-1.552127914D+03	9.803424720D+00	-2.488118587D-03	7.501565130D-07					
3.135384495D-10	-1.986281446D-13			9.137758390D+04	-2.792300566D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.847531020D+05	5.327893020D+02	6.281908900D+00	4.522790120D-04	-1.426421096D-07					
2.079708115D-11	-9.691709890D-16			7.884213810D+04	-4.216110530D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.635869714D+08	1.203460697D+05	-2.737707929D+01	4.676205400D-03	-3.035589058D-07					
9.547077170D-12	-1.181291324D-16			-8.508449070D+05	2.843901430D+02				

SF2- Chase,1998 p1145 12/76.

3	g 1/01 S	1.00F	2.00E	1.00	0.00	0.00	0	70.0623550	-394794.960
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.284572480D+04	-1.032342905D+03	1.006404631D+01	-5.209503250D-03	5.168381370D-06					
-2.783420867D-09	6.286410080D-13			-4.423303780D+04	-2.699266970D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.376618950D+04	-3.638995270D+01	7.027942820D+00	-1.142143365D-05	2.566295898D-09					
-2.981125977D-13	1.395700722D-17			-4.967050330D+04	-8.483087899D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.168882121D+04	-5.051042570D+01	7.011106220D+00	-1.262936151D-06	7.835542760D-11					
-2.517641418D-15	3.278401810D-20			-4.951246860D+04	-8.370909449D+00				

SF3 Gurvich,1989 pt1 p306 pt2 p186.

2	tpis89 S	1.00F	3.00	0.00	0.00	0.00	0	89.0602096	-504101.395
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.284008253D+05	-2.084871223D+03	1.423421102D+01	-4.015032190D-03	9.152258040D-07					
1.109809721D-09	-5.988602720D-13			-5.239517340D+04	-5.187194724D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.411283460D+05	-1.418950375D+02	1.010590548D+01	-4.231526910D-05	9.336120600D-09					
-1.068727665D-12	4.944342600D-17			-6.358445860D+04	-2.489561796D+01				

## Appendix D (continued)

SF3+ Chase,1998 p1170.

3 j12/76 S	1.00F	3.00E	-1.00	0.00	0.00	0.00	89.0596610	393583.476
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.157633857D+05	-2.564488498D+03	1.323216044D+01	-1.749580869D-04	-3.712958710D-06				
3.580688420D-09	-1.084376153D-12		5.876088420D+04	-5.024130184D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.778260750D+05	-1.621770252D+02	9.960265970D+00	1.237729568D-04	-6.442207890D-08				
1.300856025D-11	-7.915106980D-16		4.415426810D+04	-2.673900770D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.358347800D+06	2.002176210D+03	7.115714750D+00	6.563028420D-04	-5.120344380D-08				
1.781530495D-12	-2.365386482D-17		3.575488850D+04	-4.384285323D+00				

SF3- Gurvich,1989 pt1 p307 pt2 p187.

2 tpis89 S	1.00F	3.00E	1.00	0.00	0.00	0.00	89.0607582	-790124.207
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.546500675D+05	-2.469768526D+03	1.657548496D+01	-1.020137434D-02	9.368008460D-06				
-4.725672600D-09	1.009661431D-12		-8.500157900D+04	-6.532166474D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.253860964D+05	-1.308890242D+02	1.009972380D+01	-4.052345530D-05	9.064565220D-09				
-1.049320641D-12	4.899201260D-17		-9.800227200D+04	-2.524368023D+01				

SF4 Gurvich,1989 pt1 p307 pt2 p188.

2 tpis89 S	1.00F	4.00	0.00	0.00	0.00	0.00	108.0586128	-760000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.636183265D+05	-2.531316261D+03	1.559106568D+01	3.326704310D-03	-1.054935525D-05				
9.391363050D-09	-2.914816694D-12		-8.115558920D+04	-6.131532958D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.777125160D+05	-2.937595659D+02	1.321902007D+01	-8.747669450D-05	1.929905265D-08				
-2.209423506D-12	1.022335559D-16		-9.483175340D+04	-4.243061278D+01				

SF4+ Chase,1998 p1188.

3 j12/76 S	1.00F	4.00E	-1.00	0.00	0.00	0.00	108.0580642	416111.962
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.309587324D+05	-3.383777670D+03	2.101756367D+01	-1.106529555D-02	9.038097280D-06				
-4.055912640D-09	7.12575180D-13		6.425375150D+04	-8.938224908D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.189172750D+05	4.002889640D+01	1.283873264D+01	1.340235036D-04	-4.818135180D-08				
7.574595960D-12	-3.696670780D-16		4.469944230D+04	-3.760378598D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.761690270D+07	2.881726011D+04	4.470948840D+00	1.170801362D-03	-7.325658000D-08				
2.214151827D-12	-2.649348632D-17		-1.772949712D+05	3.397688982D+01				

SF4- Chase,1998 p1189.

3 j12/76 S	1.00F	4.00E	1.00	0.00	0.00	0.00	108.0591614	-887464.320
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.005523355D+05	-2.267351994D+03	1.979284560D+01	-1.163761842D-02	1.161792139D-05				
-6.288895470D-09	1.426371272D-12		-9.895597430D+04	-7.916366078D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.208822080D+05	-1.710416599D+03	1.494425485D+01	-1.057207329D-03	2.742846920D-07				
-2.905761211D-11	1.084482543D-15		-1.005231225D+05	-5.164256578D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.436095670D+07	-3.546125020D+04	2.105391090D+01	-7.366819310D-04	3.537247530D-08				
-8.825254090D-13	9.049180280D-18		1.694175033D+05	-1.089710894D+02				

SF5 Gurvich,1989 pt1 p308 pt2 p189.

2 tpis89 S	1.00F	5.00	0.00	0.00	0.00	0.00	127.0570160	-902663.287
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.224176850D+05	-4.043991750D+03	2.707196786D+01	-1.744176604D-02	1.604198715D-05				
-7.997243020D-09	1.667968061D-12		-9.220078270D+04	-1.232426279D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.892426370D+05	-1.825826536D+02	1.613765057D+01	-5.544834230D-05	1.231433706D-08				
-1.417173409D-12	6.584889400D-17		-1.135671054D+05	-5.577524201D+01				

SF5+ Chase,1998 p1200.

3 j12/77 S	1.00F	5.00E	-1.00	0.00	0.00	0.00	127.0564674	172644.006
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.777135620D+05	-5.646075120D+03	3.049404270D+01	-2.176488368D-02	1.941993792D-05				
-9.556201140D-09	2.000077302D-12		4.592204810D+04	-1.489889627D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.814342320D+05	7.208817390D+02	1.564386818D+01	-2.452519972D-04	2.241690996D-07				
-3.990035890D-11	2.279087545D-15		9.090953190D+03	-5.531460631D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.063623020D+06	-8.079630910D+03	1.805068495D+01	-2.624346278D-05	-4.739171840D-09				
2.144486076D-13	-2.737984333D-18		7.597515770D+04	-7.692263871D+01				

## Appendix D (continued)

SF5- Gurvich,1989 pt1 p309 pt2 p190.

2 tpis89 S	1.00F	5.00E	1.00	0.00	0.00	0	127.0575646	-1204622.287
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.095031134D+05	-3.930081140D+03	2.702127215D+01	-1.792973203D-02	1.718122152D-05				
-9.000560190D-09	1.988018147D-12		-1.291816581D+05	-1.231672857D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.733219200D+05	-1.793729521D+02	1.613699748D+01	-5.577539970D-05	1.249477046D-08				
-1.448104799D-12	6.767462300D-17		-1.498554401D+05	-5.631439391D+01				

SF6 Gurvich,1989 pt1 p311 pt2 p191.

2 tpis89 S	1.00F	6.00	0.00	0.00	0.00	0	146.0554192	-1219400.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.309526740D+05	-4.737685050D+03	2.247738068D+01	1.046954309D-02	-2.560641961D-05				
2.153716967D-08	-6.516098960D-12		-1.255360583D+05	-1.091760145D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.306726500D+05	-6.367056550D+02	1.947442853D+01	-1.894325671D-04	4.178722830D-08				
-4.783744950D-12	2.213516129D-16		-1.510609837D+05	-8.147574587D+01				

SF6- Chase,1998 p1206.

3 j 6/77 S	1.00F	6.00E	1.00	0.00	0.00	0	146.0559678	-1341876.033
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.985809210D+05	-6.934445740D+03	3.441318330D+01	-1.984032360D-02	1.497871222D-05				
-6.133234650D-09	1.045159581D-12		-1.297069066D+05	-1.747984495D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.818073510D+05	-5.947429960D+02	1.945009842D+01	-1.820212649D-04	4.057079570D-08				
-4.683820930D-12	2.182263999D-16		-1.658902452D+05	-7.965845887D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.777074958D+05	-6.533730340D+02	1.914322537D+01	-1.624883879D-05	1.006454127D-09				
-3.230395820D-14	4.203897370D-19		-1.646993323D+05	-7.753346267D+01				

SH D0:Continetti,1991. Gurvich,1989 pt1 p296 pt2 p179.

2 g10/01 S	1.00H	1.00	0.00	0.00	0.00	0	33.0729400	142135.309
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.389434680D+03	-3.747960920D+02	7.548145770D+00	-1.288875477D-02	1.907786343D-05				
-1.265033728D-08	3.235158690D-12		1.742902395D+04	-1.760761843D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.682631601D+06	-5.177152210D+03	9.198168520D+00	-2.323550224D-03	6.543914780D-07				
-4.68470420D-11	3.864741550D-15		4.899214490D+04	-3.770400275D+01				

SH- Gurvich,1989 pt1 p297 pt2 p180.

2 g10/01 S	1.00H	1.00E	1.00	0.00	0.00	0	33.0734886	-86574.096
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.878070760D+04	-5.742590600D+02	6.898544460D+00	-1.001352412D-02	1.486460572D-05				
-9.750368900D-09	2.446909813D-12		-8.735388980D+03	-1.615966489D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.198715402D+06	-3.894846820D+03	7.660422330D+00	-1.355237590D-03	3.342370240D-07				
-3.350722310D-11	9.055084780D-16		1.317477387D+04	-2.818370616D+01				

SN Gurvich,1989 pt1 p392 pt2 p252.

2 tpis89 S	1.00N	1.00	0.00	0.00	0.00	0	46.0717000	267388.313
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.835412350D+04	1.147567483D+03	-2.877802574D+00	1.724864320D-02	-2.058999904D-05				
1.261369640D-08	3.139030141D-12		2.564143612D+04	4.224006964D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.837284460D+05	1.058075590D+03	3.086198804D+00	9.111360780D-04	-2.764061722D-07				
4.157370110D-11	-2.128351755D-15		2.379345477D+04	1.033222139D+01				

SO Gurvich,1989 pt1 p286 pt2 p173.

2 tpis89 S	1.000	1.00	0.00	0.00	0.00	0	48.0644000	4760.306
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.342757000D+04	6.403862500D+02	-1.006641228D+00	1.381512705D-02	-1.704486364D-05				
1.061294930D-08	-2.645796205D-12		-3.371292190D+03	3.093861963D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.443410557D+06	4.113874360D+03	-5.383695780D-01	2.794153269D-03	-6.633352260D-07				
7.838221190D-11	-3.560509070D-15		-2.708838059D+04	3.615358329D+01				

SO- Gurvich,1989 pt1 p288 pt2 p174.

2 tpis89 S	1.000	1.00E	1.00	0.00	0.00	0	48.0649486	-105968.086
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.420196970D+03	-6.916586680D+01	3.837666610D+00	2.166482062D-03	-2.811222562D-06				
1.793426453D-09	-4.521795950D-13		-1.354162531D+04	4.316141603D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.767156147D+05	-6.633987360D+02	5.177279810D+00	-2.853461125D-04	7.214421530D-08				
-3.676469490D-12	-2.910092894D-16		-9.984438010D+03	-3.951456757D+00				

## Appendix D (continued)

SOF2                      Gurvich,1989 pt1 p312 pt2 p192.

2 tps89 S	1.000	1.00F	2.00	0.00	0.00	0.00	0.00	86.0612064	-584952.313
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.114579650D+04	-9.081119670D+02	6.883623260D+00	1.192459695D-02	-1.671006410D-05					
1.110723646D-08	-2.910788226D-12							-6.742935840D+04	-1.125458745D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.510555779D+05	-6.074439610D+02	1.045046709D+01	-1.796384979D-04	3.964169730D-08					
-4.543055240D-12	2.104969923D-16							-7.072071710D+04	-2.904334504D+01

SO2                      Gurvich,1989 pt1 p288 pt2 p175.

2 tps89 S	1.000	2.00	0.00	0.00	0.00	0.00	0.00	64.0638000	-296810.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.310842140D+04	9.090311670D+02	-2.356891244D+00	2.204449885D-02	-2.510781471D-05					
1.446300484D-08	-3.369070940D-12							-4.113752080D+04	4.045512519D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.127640116D+05	-8.252261380D+02	7.616178630D+00	-1.999327610D-04	5.655631430D-08					
-5.454316610D-12	2.104969923D-16							-3.351308690D+04	-1.655776085D+01

SO2-                      Gurvich,1989 pt1 p290 pt2 p176.

2 tps89 S	1.000	2.00E	1.00	0.00	0.00	0.00	0.00	64.0643486	-408606.069
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.460901660D+04	-8.562691050D+02	5.360074220D+00	7.609576740D-03	-1.092005659D-05					
7.202547730D-09	-1.850138220D-12							-4.580094810D+04	-3.929956604D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.793400005D+05	-3.663168760D+02	7.274441050D+00	-1.101944663D-04	2.443328132D-08					
-2.809735019D-12	1.305160431D-16							-4.973072610D+04	-1.261421156D+01

SO2CL2                      Chase,1998 p847.

2 j 6/71 S	1.000	2.00CL	2.00	0.00	0.00	0.00	0.00	134.9698000	-354803.200
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.821592390D+03	-5.849569200D+02	8.596756910D+00	1.197228675D-02	-1.333760700D-05					
7.126129000D-09	-1.496150016D-12							-4.230783810D+04	-1.652458363D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.376639109D+05	-9.647740410D+02	1.371469904D+01	-2.850327057D-04	6.293509620D-08					
-7.217844260D-12	3.346840220D-16							-4.190072990D+04	-4.481942575D+01

SO2FCL                      Chase,1998 p754.

2 j 6/71 S	1.000	2.00F	1.00CL	1.00	0.00	0.00	0.00	118.5152032	-556472.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.684561300D+04	-8.038358950D+02	7.526186880D+00	1.620141782D-02	-1.970595270D-05					
1.166250330D-08	-2.759241465D-12							-6.503598190D+04	-1.299745646D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.915402438D+05	-1.107134423D+03	1.381845158D+01	-3.258514460D-04	7.184741000D-08					
-8.230625200D-12	3.812925620D-16							-6.552472690D+04	-4.709166446D+01

SO2F2                      Gurvich,1989 pt1 p313 pt2 p193.

2 tps89 S	1.000	2.00F	2.00	0.00	0.00	0.00	0.00	102.0606064	-760000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.533153530D+04	-8.074639680D+02	5.287172160D+00	2.294547775D-02	-2.891025299D-05					
1.785631907D-08	-4.418919500D-12							-8.899428820D+04	-4.124256607D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.403904450D+05	-1.309288764D+03	1.396601541D+01	-3.840088150D-04	8.456688780D-08					
-9.678246870D-12	4.480014280D-16							-8.901994140D+04	-5.109270050D+01

SO3                      Gurvich,1989 pt1 p292 pt2 p177.

2 tps89 S	1.000	3.00	0.00	0.00	0.00	0.00	0.00	80.0632000	-395900.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.952855290D+04	6.208572570D+02	-1.437731716D+00	2.764126467D-02	-3.144958662D-05					
1.792798000D-08	-4.126386660D-12							-5.184106170D+04	3.391331216D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.166923781D+05	-1.301022399D+03	1.096287985D+01	-3.837100020D-04	8.466889040D-08					
-9.705399290D-12	4.498397540D-16							-4.398283990D+04	-3.655217314D+01

S2                      Gurvich,1989 pt1 p270 pt2 p165.

2 tps89 S	2.00	0.00	0.00	0.00	0.00	0.00	0.00	64.1300000	128600.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.528091780D+04	-4.222156580D+02	4.677433490D+00	1.724046361D-03	-3.862208210D-06					
3.336156340D-09	-9.930661540D-13							1.654767715D+04	-7.957279032D-01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.588128788D+04	6.315480880D+02	2.449628069D+00	1.986240565D-03	-6.507927240D-07					
1.002813651D-10	-5.596990050D-15							1.085508427D+04	1.458544515D+01

## Appendix D (continued)

S2- Gurvich,1989 pt1 p274 pt2 p166.

2	tpis89 S	2.00E	1.00	0.00	0.00	0.00	0	64.1305486	-37132.385
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.025558251D+04	-6.166128250D+02	8.182052840D+00	-8.311203580D-03	9.720274160D-06					
-5.775476780D-09	1.393690695D-12							-3.063559874D+03	-1.906068041D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.830204030D+05	-1.319171302D+03	6.031778480D+00	-7.965560690D-04	2.282241690D-07					
-2.504364698D-11	7.280550780D-16							2.660258490D+03	-9.010480319D+00

S2CL2 Chase,1998 p859 6/78.

2	g12/00 S	2.00CL	2.00	0.00	0.00	0.00	0	135.0360000	-16736.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.974974740D+04	-1.636770024D+03	1.583744686D+01	-1.186906072D-02	1.413008027D-05					
-8.484903930D-09	1.981743887D-12							3.276872420D+03	-5.293745205D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.328816000D+05	-3.442705800D+03	1.519637350D+01	-2.960877176D-03	6.888284370D-07					
-7.990692530D-13	3.692466060D-15							1.526672656D+04	-5.453315445D+01

S2F2 Thiothionyl fluoride. Chase,1998 p1147.

2	j 6/76 S	2.00F	2.00	0.00	0.00	0.00	0	102.1268064	-401413.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.252904041D+05	-1.941243874D+03	1.325382183D+01	-1.341525124D-03	-2.772465632D-06					
3.658169290D-09	-1.299531209D-12							-4.067208250D+04	-4.560828617D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.591757719D+05	-1.059653069D+02	1.006588551D+01	-2.274618148D-05	5.412343140D-09					
-9.911387140D-13	9.621861440D-17							-5.147675180D+04	-2.375666140D+01

S2O Gurvich,1989 pt1 p293 pt2 p178.

2	tpis89 S	2.000	1.00	0.00	0.00	0.00	0	80.1294000	-56035.495
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.092703310D+04	-9.523099870D+01	3.144525430D+00	1.176854200D-02	-1.580266840D-05					
1.037645040D-08	-2.708622260D-12							-7.500471900D+03	1.104169896D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.442139790D+05	-3.276430130D+02	7.244286110D+00	-9.776538300D-05	2.162712700D-08					
-2.482782220D-12	1.151778750D-16							-7.438553930D+03	-1.085180744D+01

S3 Gurvich,1989 pt1 p275 pt2 p167.

2	tpis89 S	3.00	0.00	0.00	0.00	0.00	0	96.1950000	144738.328
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.245395740D+04	-1.162146759D+03	9.955413680D+00	-4.158026220D-03	3.241778390D-06					
-1.264648239D-09	1.777450535D-13							2.146275475D+04	-2.587525865D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.117805401D+05	-5.197908390D+01	7.038760840D+00	-1.546804022D-05	3.408340410D-09					
-3.896862360D-13	1.800860389D-17							1.525406485D+04	-7.610045099D+00

S4 Gurvich,1989 pt1 p280 pt2 p168.

2	tpis89 S	4.00	0.00	0.00	0.00	0.00	0	128.2600000	135632.333
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.198664135D+05	-2.040786521D+03	1.510235054D+01	-7.041104300D-03	5.350405000D-06					
-2.002348038D-09	2.569940995D-13							2.410909409D+04	-5.503153238D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.068333537D+05	-9.696151430D+01	1.007243210D+01	-2.895047053D-05	6.387806190D-09					
-7.311767430D-13	3.382265290D-17							1.321109530D+04	-2.344872237D+01

S5 Gurvich,1989 pt1 p281 pt2 p169.

2	tpis89 S	5.00	0.00	0.00	0.00	0.00	0	160.3250000	132993.354
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.361370439D+05	-2.955476536D+03	2.633358816D+01	-4.125806530D-02	7.056814030D-05					
-5.611095330D-08	1.659457200D-11							2.675307046D+04	-1.069711067D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.038495160D+06	8.601803880D+03	7.443780900D+00	1.533393812D-03	-2.532718676D-07					
2.145210795D-11	7.213102680D-16							-4.686925420D+04	1.104229196D+01

S6 Gurvich,1989 pt1 p282 pt2 p170.

2	tpis89 S	6.00	0.00	0.00	0.00	0.00	0	192.3900000	101315.180
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.780307210D+04	-2.568470130D+03	2.467025557D+01	-1.619983175D-02	1.712334526D-05					
-9.746296740D-09	2.486964867D-12							2.037888389D+04	-1.014410309D+02
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.686845060D+06	-7.695017900D+03	1.860721995D+01	2.290382548D-03	-1.219834021D-06					
2.060780798D-10	-1.190354318D-14							6.032486480D+04	-7.490245718D+01



## Appendix D (continued)

S7 Gurvich,1989 pt1 p283 pt2 p171.  
 2 tpis89 S 7.00 0.00 0.00 0.00 0.00 0.00 0 224.4550000 111890.369  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26274.368  
 1.233655613D+05-3.200543640D+03 3.015678887D+01-2.197472483D-02 2.487892075D-05  
 -1.506049557D-08 3.768925990D-12 2.390005896D+04-1.275978171D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26274.368  
 -2.726396041D+05-7.373215220D+01 1.905771987D+01-2.394575885D-05 5.442671300D-09  
 -6.379663480D-13 3.008212993D-17 7.308458830D+03-6.159112428D+01

S8 Gurvich,1989 pt1 p284 pt2 p172.  
 2 tpis89 S 8.00 0.00 0.00 0.00 0.00 0 256.5200000 101277.122  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31573.122  
 3.145625719D+05-6.116510160D+03 4.875327540D+01-6.241794650D-02 7.421831750D-05  
 -3.726449310D-08 5.799429880D-12 3.573890840D+04-2.288701977D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31573.122  
 -8.727921130D+06 1.221627968D+04 2.209959617D+01-3.494064830D-03 1.397604162D-06  
 -2.169815281D-10 1.212304364D-14 -8.658110820D+04-6.435742508D+01

Sc Hf:Gurvich,1982. Sugar,1985. Gordon,1999.  
 3 g 1/99 SC 1.00 0.00 0.00 0.00 0.00 0 44.9559100 377700.259  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7002.259  
 -3.700805940D+03 1.692506026D+02 1.842242597D+00 1.364835821D-03-1.580085847D-06  
 9.613111150D-10-2.392381918D-13 4.385215240D+04 1.072781921D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7002.259  
 8.810382650D+06-2.711232975D+04 3.476588660D+01-1.861104581D-02 5.290283900D-06  
 -6.585408060D-10 2.997850429D-14 2.162460097D+05-2.225618519D+02  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7002.259  
 2.283130511D+09-1.367701232D+06 3.213593060D+02-3.563171100D-02 2.093254715D-06  
 -6.238650020D-11 7.425605615D-16 1.092708359D+07-2.781409383D+03

Sc+ Sugar,1985. Gordon,1999.  
 3 g 7/97 SC 1.00E -1.00 0.00 0.00 0.00 0 44.9553614 1017145.222  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7161.922  
 -5.884930160D+03 1.479044408D+02 2.009576456D+00 7.389566970D-04-6.617964820D-07  
 6.841073760D-10-2.164125532D-13 1.208439139D+05 1.026570620D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7161.922  
 1.973658531D+06-4.954384100D+03 6.360627350D+00-7.168785920D-04 2.464991123D-08  
 9.632373790D-12-8.544709642D-16 1.543423764D+05-2.261925782D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7161.922  
 2.219151811D+08-1.287881370D+05 3.265593870D+01-3.379963200D-03 1.981741972D-07  
 -5.190207160D-12 4.635586113D-17 1.149364313D+06-2.553294937D+02

Sc- Hotop,1985. Used J from isoelectronic Ti. Gordon,1999.  
 3 g 9/97 SC 1.00E 1.00 0.00 0.00 0.00 0 44.9564586 352558.828  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 4.165746390D+04 8.270420720D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 4.165746390D+04 8.270420720D+00  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 0.000000000D+00 0.000000000D+00 2.500000000D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 4.165746390D+04 8.270420720D+00

ScO D0,Props(extrap):Gurvich,1982 pt1 p140 pt2 p143.  
 3 tpis89 SC 1.000 1.00 0.00 0.00 0.00 0 60.9553100 -55065.294  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8787.106  
 -3.136784613D+03 2.271981685D+02 8.850757320D-01 1.052430774D-02-1.431954596D-05  
 9.652351070D-09-2.586210633D-12 -8.550798770D+03 2.012706847D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8787.106  
 1.224192443D+06-3.918915720D+03 8.679848810D+00-1.995893306D-03 4.066989850D-07  
 -1.504459913D-11-8.472998900D-16 1.677322594D+04-2.951656272D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8787.106  
 5.435720930D+08-2.629571561D+05 4.324788690D+01-8.590816240D-04-1.205059380D-07  
 6.918221540D-12-1.109417319D-16 2.162498313D+06-3.650332350D+02

ScO+ D0,Estim.cons:Gurvich,1982 pt1 p142 pt2 p145.  
 3 g10/99 SC 1.000 1.00E -1.00 0.00 0.00 0 60.9547614 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

## Appendix D (continued)

ScO2 Gurvich,1982 pt1 p143 pt2 p147.

2	tpis82 SC	1.000	2.00	0.00	0.00	0.00	0	76.9547100	-413650.667
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.794700960D+04	-4.298358590D+02	3.417206500D+00	1.361338544D-02	-2.047465023D-05					
1.455906041D-08	-4.038087690D-12		-4.861049530D+04	7.670013330D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.903902542D+05	-2.315588820D+02	7.172104910D+00	-6.859209640D-05	1.510998557D-08					
-1.727951588D-12	7.988980500D-17		-5.112974750D+04	-1.090764597D+01					

Sc2O Gurvich,1982 pt1 p144 pt2 p148.

2	tpis82 SC	2.000	1.00	0.00	0.00	0.00	0	105.9112200	-23044.208
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.550002615D+04	-3.077608607D+02	4.671215040D+00	8.696142250D-03	-1.283873116D-05					
8.988966810D-09	-2.461994147D-12		-2.614951944D+03	2.920017180D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.350880396D+05	-1.854540692D+02	7.138294080D+00	-5.529432140D-05	1.221589315D-08					
-1.400490463D-12	6.488858110D-17		-4.240235140D+03	-9.372710950D+00					

Sc2O2 Gurvich,1982 pt1 p145 pt2 p149.

2	tpis82 SC	2.000	2.00	0.00	0.00	0.00	0	121.9106200	-490571.020
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.468445490D+03	2.617988314D+02	-3.052099624D-01	3.076104070D-02	-4.183478360D-05					
2.794218425D-08	-7.412672050D-12		-6.144013210D+04	2.915248555D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.977348677D+05	-5.803677920D+02	1.043318377D+01	-1.734165462D-04	3.836089790D-08					
-4.403078030D-12	2.042208922D-16		-5.964866280D+04	-2.855828369D+01					

Si Hf:Cox,1989. NIST data version1.1 [Online]1997. Gordon,1999.

3	g 8/97 SI	1.00	0.00	0.00	0.00	0.00	0	28.0855000	450000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.836140810D+01	1.546544523D+02	1.876436670D+00	1.320637995D-03	-1.529720059D-06					
8.950562770D-10	-1.952873490D-13		5.263510310D+04	9.698288880D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.169298850D+05	2.240683927D+03	-4.448619320D-01	1.710056321D-03	-4.107714160D-07					
4.558884780D-11	-1.889515353D-15		3.953558760D+04	2.679668061D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.286548940D+08	5.443989890D+05	-1.206739736D+02	1.359662698D-02	-7.606498660D-07					
-2.149746065D-11	-2.474116774D-16		-4.293792120D+06	1.086382839D+03					

Si+ Martin,1983. Gordon,1999.

3	g 4/97 SI	1.00E	-1.00	0.00	0.00	0.00	0	28.0849514	1242508.045
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.329791880D+04	6.795894490D+02	2.257046144D-01	4.118600490D-03	-4.234881600D-06					
2.327995626D-09	-5.318388059D-13		1.452039813D+05	1.934650510D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.919390230D+04	-4.856730950D+01	2.556312024D+00	-3.503397160D-05	1.190298787D-08					
-2.082923821D-12	1.471452049D-16		1.491431392D+05	5.244267140D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.364077210D+07	2.434350601D+04	-2.763336522D+00	5.924483200D-04	-4.454048310D-08					
2.509351585D-12	-5.090212919D-17		-4.683214410D+04	5.196564190D+01					

Si- Chase,1998 p1887 3/83. EA:Hotop,1985. Gordon,1999.

3	g 4/97 SI	1.00E	1.00	0.00	0.00	0.00	0	28.0860486	308817.528
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.940146670D+02	5.567418420D+00	2.499837183D+00	-9.481394460D-05	3.171246930D-07					
-4.191323180D-10	2.035924380D-13		3.636443380D+04	5.270119840D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.162070100D+06	1.883310402D+04	-1.899302450D+01	1.111021657D-02	-2.535790208D-06					
2.699962923D-10	-1.105062911D-14		-8.314089310D+04	1.595298253D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.429517960D+07	3.297105700D+04	-2.470579690D+00	3.966577600D-04	-1.764141255D-08					
4.115769760D-13	-3.904369380D-18		-2.315881505D+05	5.226601830D+01					

SiBr Gurvich,1991 pt1 p280 pt2 p249.

2	tpis91 SI	1.00BR	1.00	0.00	0.00	0.00	0	107.9895000	175157.421
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.370283350D+03	-5.051062960D+02	8.280591040D+00	-1.005383920D-02	1.357050920D-05					
-9.115449900D-09	2.447477685D-12		2.184405475D+04	-1.662032657D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.317799940D+06	-3.669795020D+03	8.511686120D+00	-1.987602041D-03	5.035414890D-07					
-4.490120190D-11	8.235670070D-16		4.332851550D+04	-2.467075472D+01					

## Appendix D (continued)

SiBr2                      Gurvich,1991 pt1 p281 pt2 p250.

2 tps91 SI	1.00BR	2.00	0.00	0.00	0.00	0	187.8935000	-51000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.386616151D+04	-6.415693470D+02	9.345879110D+00	-4.792904140D-03	5.582538470D-06				
-3.455312380D-09	8.800338940D-13		-5.014757020D+03	-1.740767596D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.147343940D+04	-1.277719997D+01	7.010202240D+00	-4.296331860D-06	9.877651970D-10				
-1.168133105D-13	5.546681380D-18		-8.319542250D+03	-3.611826610D+00				

SiBr3                      Gurvich,1991 pt1 p282 pt2 p251.

2 tps91 SI	1.00BR	3.00	0.00	0.00	0.00	0	267.7975000	-157000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.972806860D+04	-1.066475023D+03	1.380836232D+01	-7.641114720D-03	8.775865830D-06				
-5.372430850D-09	1.356453455D-12		-1.651795623D+04	-3.784055370D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.888024740D+04	-2.267879074D+01	1.001791167D+01	-7.481150750D-06	1.709242690D-09				
-2.011596627D-13	9.515534150D-18		-2.203026938D+04	-1.537574366D+01				

SiBr4                      Gurvich,1991 pt1 p283 pt2 p252.

2 tps91 SI	1.00BR	4.00	0.00	0.00	0.00	0	347.7015000	-415800.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.821086740D+04	-1.520370776D+03	1.810453360D+01	-9.734688420D-03	1.072367466D-05				
-6.343858290D-09	1.557228200D-12		-4.616585210D+04	-5.976120630D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.271409281D+05	-3.768087950D+01	1.302910642D+01	-1.194958251D-05	2.693843051D-09				
-3.137193207D-13	1.471642663D-17		-5.408998830D+04	-2.940384330D+01				

SiC                        Gurvich,1991 pt1 p301 pt2 p265.

2 tps91 SI	1.00C	1.00	0.00	0.00	0.00	0	40.0962000	734946.140
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.223330890D+03	3.141790457D+02	3.893130830D-01	1.187507540D-02	-1.639277197D-05				
1.131808223D-08	-3.045324231D-12		8.606227730D+04	2.310166717D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.268806030D+04	7.209836920D+02	2.162879732D+00	2.201299585D-03	-6.569466590D-07				
9.177110260D-11	4.969166740D-15		8.321225850D+04	1.601675317D+01				

SiC2                      Gurvich,1991 pt1 p302 pt2 p266.

2 tps91 SI	1.00C	2.00	0.00	0.00	0.00	0	52.1069000	631360.938
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.119628990D+04	6.869747180D+02	2.361343691D-02	1.532939217D-02	-1.435588838D-05				
6.375228740D-09	-1.059204957D-12		7.130890710D+04	2.828850316D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.026893090D+06	-2.466148437D+04	3.915453030D+01	-2.002884068D-02	6.307353690D-06				
-8.848383510D-10	4.530549850D-14		2.267325155D+05	-2.366622024D+02				

SiCL                      Gurvich,1991 pt1 p271 pt2 p243.

2 tps91 SI	1.00CL	1.00	0.00	0.00	0.00	0	63.5385000	142363.219
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.248508319D+04	-2.044170347D+02	4.977070850D+00	-5.160756260D-04	2.931980374D-07				
-3.666615230D-12	-3.393037130D-14		1.686528019D+04	-2.263957240D-01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.767294560D+05	-1.147956509D+03	5.735408430D+00	-5.784890810D-04	1.517304648D-07				
-1.291391394D-11	1.554628420D-16		2.306278401D+04	-6.098515228D+00				

SiCL2                     Gurvich,1991 pt1 p273 pt2 p244.

2 tps91 SI	1.00CL	2.00	0.00	0.00	0.00	0	98.9915000	-163069.287
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.305550970D+04	-1.015842786D+03	1.032848185D+01	-6.212267520D-03	6.715825400D-06				
-3.908801640D-09	9.461732150D-13		-1.650218093D+04	-2.649925756D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.050871570D+04	-2.661025523D+01	7.020414720D+00	-8.335824720D-06	1.871092411D-09				
-2.171552767D-13	1.015849895D-17		-2.181294885D+04	-6.638764238D+00				

SiCL3                     Gurvich,1991 pt1 p275 pt2 p245.

2 tps91 SI	1.00CL	3.00	0.00	0.00	0.00	0	134.4445000	-336271.670
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.691708460D+04	-1.677556857D+03	1.511519060D+01	-8.937031000D-03	9.097353530D-06				
-5.014579960D-09	1.155962016D-12		-3.477477300D+04	-5.087215506D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.477180114D+05	-5.335200980D+01	1.004043521D+01	-1.635121060D-05	3.641940110D-09				
-4.200600590D-13	1.955201587D-17		-4.360571650D+04	-2.006632444D+01				

## Appendix D (continued)

SiCL4 Gurvich,1991 pt1 p276 pt2 p246.

2 tps91 SI	1.00CL	4.00	0.00	0.00	0.00	0.00	0	169.8975000	-662200.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.171646285D+05	-2.185821461D+03	1.908250496D+01	-9.636335720D-03	8.836847690D-06					
-4.360042400D-09	8.940232430D-13		-7.212802110D+04	-7.301532221D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.100330761D+05	-8.476107710D+01	1.306364027D+01	-2.554020420D-05	5.653818470D-09					
-6.488752670D-13	3.008025543D-17		-8.372268130D+04	-3.592584781D+01					

SiF Gurvich,1991 pt1 p264 pt2 p238.

2 tps91 SI	1.00F	1.00	0.00	0.00	0.00	0	47.0839032	-25232.686
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.478223768D+04	1.357998649D+01	2.324182643D+00	7.132851180D-03	-1.022951215D-05				
7.148396470D-09	-1.964689785D-12		-3.995380650D+03	1.231128121D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.653637880D+05	8.722860040D+02	3.377218270D+00	7.508152430D-04	-2.308898619D-07				
3.766781800D-11	-2.143080403D-15		-1.011697664D+04	8.968132820D+00				

SiFCL Gurvich,1991 pt1 p279 pt2 p248.

2 tps91 SI	1.00F	1.00CL	1.00	0.00	0.00	0	82.5369032	-377826.516
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.176954640D+04	-5.926575380D+02	6.409770710D+00	4.641682610D-03	-7.978461910D-06				
6.008728370D-09	-1.720953157D-12		-4.398296070D+04	-6.259737448D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.284698945D+05	-1.247550173D+02	7.092893850D+00	-3.707311770D-05	8.175173010D-09				
-9.356435210D-13	4.328544340D-17		-4.723309720D+04	-8.337392708D+00				

SiF2 Gurvich,1991 pt1 p266 pt2 p239.

2 tps91 SI	1.00F	2.00	0.00	0.00	0.00	0	66.0823064	-592838.108
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.053236650D+04	-3.997637560D+02	4.055303880D+00	1.153423049D-02	-1.757586754D-05				
1.260369111D-08	-3.517105220D-12		-7.047770460D+04	3.879854420D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.675200202D+05	-1.846212090D+02	7.136986350D+00	-5.450769860D-05	1.199012961D-08				
-1.369470187D-12	6.324889990D-17		-7.287401020D+04	-1.117933348D+01				

SiF3 Gurvich,1991 pt1 p268 pt2 p240

2 tps91 SI	1.00F	3.00	0.00	0.00	0.00	0	85.0807096	-996436.577
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.755369980D+04	-7.179595770D+02	5.379396940D+00	1.813065142D-02	-2.738373356D-05				
1.946519470D-08	-5.390790560D-12		-1.177631169D+05	-3.442902040D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.903283702D+05	-3.427876940D+02	1.025536335D+01	-1.019796690D-04	2.250326132D-08				
-2.577117181D-12	1.192923177D-16		-1.218088967D+05	-2.725261142D+01				

SiF4 Johnson,1986. McDowell,1982. Chase,1998 p1190 (6/76).

2 g 6/01 SI	1.00F	4.00	0.00	0.00	0.00	0	104.0791128	-1615780.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.069670784D+04	-9.569638640D+01	2.513988593D+00	3.309781030D-02	-4.573044080D-05				
3.091834452D-08	-8.269304050D-12		-1.956252529D+05	1.133722022D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.845892320D+05	-6.569979910D+02	1.348925720D+01	-5.100471360D-05	5.346329580D-08				
-4.959598110D-12	2.299314375D-16		-1.957284479D+05	-4.673894650D+01				

SiH Gurvich,1991 pt1 p257 pt2 p234.

2 tps91 SI	1.00H	1.00	0.00	0.00	0.00	0	29.0934400	368636.210
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.426676300D+03	7.417251210D+01	3.973491600D+00	-4.149408880D-03	1.022918384D-05				
-8.592386360D-09	2.567093743D-12		4.281745800D+04	2.246937150D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.042086490D+05	-2.364796524D+03	7.627499140D+00	-2.496591233D-03	1.108436410D-06				
-1.943991955D-10	1.136251507D-14		5.704737680D+04	-2.448054429D+01				

SiH+ Chase,1998 p1308.

2 j12/71 SI	1.00H	1.00E	-1.00	0.00	0.00	0	29.0928914	1147671.167
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.307157170D+04	3.884958240D+02	2.546166863D+00	-6.686325980D-04	5.186277020D-06				
-4.818569740D-09	1.445702640D-12		1.349079707D+05	9.027950090D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.711692033D+05	-1.045807287D+03	4.838648240D+00	1.277940891D-04	-6.883872450D-08				
1.418843480D-11	-7.855316960D-16		1.431721450D+05	-7.553299140D+00				

## Appendix D (continued)

SiHBr3 Chase,1998 p514.  
 2 j12/76 SI 1.00H 1.00BR 3.00 0.00 0.00 0 268.8054400 -302922.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17823.429  
 1.322811122D+05-2.205365507D+03 1.775084194D+01-1.047794569D-02 1.286821723D-05  
 -7.743124260D-09 1.819060891D-12 -2.834992682D+04-6.331199540D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17823.429  
 2.199973526D+05-2.024458552D+03 1.435781007D+01-5.037015840D-04 1.054049755D-07  
 -1.160828765D-11 5.217257680D-16 -2.842086214D+04-4.536437170D+01

SiHCL Gurvich,1991 pt1 p277 pt2 p247.  
 2 tpis91 SI 1.00H 1.00CL 1.00 0.00 0.00 0 64.5464400 54945.913  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10665.413  
 5.909673050D+04-8.780064030D+02 7.999687930D+00-4.663141270D-03 8.594986000D-06  
 -6.608073550D-09 1.868076396D-12 9.567570340D+03-1.690014311D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10665.413  
 1.012152890D+05-1.163239598D+03 7.376366550D+00 1.874151313D-04-1.661351093D-07  
 3.964414040D-11-2.640580080D-15 1.141064087D+04-1.507678798D+01

SiHCL3 Chase,1998 880.  
 2 j12/76 SI 1.00H 1.00CL 3.00 0.00 0.00 0 135.4524400 -496222.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16151.608  
 1.659565586D+05-2.552498122D+03 1.750117375D+01-7.885728660D-03 8.092567490D-06  
 -3.980420600D-09 7.059173320D-13 -4.951316600D+04-6.758519053D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16151.608  
 1.728644072D+05-2.116727327D+03 1.441802307D+01-5.255249620D-04 1.098826178D-07  
 -1.209327059D-11 5.432187050D-16 -5.130351940D+04-5.036360893D+01

SiHF Gurvich,1991 pt1 p270 pt2 p242.  
 2 tpis91 SI 1.00H 1.00F 1.00 0.00 0.00 0 48.0918432 -162657.169  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10230.231  
 2.192598671D+04-6.175229080D+01 2.127372739D+00 1.123538312D-02-1.322503985D-05  
 8.307307390D-09-2.010545971D-12 -2.016994845D+04 1.367184876D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10230.231  
 4.049752240D+06-9.295526820D+03 1.071754366D+01 1.868124220D-03-1.129820372D-06  
 1.960250100D-10-1.144682011D-14 4.133225200D+04-4.736317600D+01

SiHF3 Chase,1998 p1160.  
 2 j 6/76 SI 1.00H 1.00F 3.00 0.00 0.00 0 86.0886496 -1200808.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13544.634  
 8.325879390D+04-8.178594460D+02 4.041717240D+00 2.726104628D-02-3.787831480D-05  
 2.630589305D-08-7.289582500D-12 -1.416146961D+05 1.382806532D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13544.634  
 7.820100800D+04-2.592742261D+03 1.475104214D+01-6.531047200D-04 1.372428937D-07  
 -1.516371051D-11 6.832497150D-16 -1.336611887D+05-5.851450950D+01

SiHI3 Chase,1998 p1266.  
 2 j12/76 SI 1.00H 1.00I 3.00 0.00 0.00 0 409.8068500 -74475.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19135.424  
 1.113840054D+05-1.974457175D+03 1.791396249D+01-1.219208519D-02 1.613169233D-05  
 -1.038096942D-08 2.613287761D-12 -2.256377425D+03-5.995455130D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19135.424  
 2.279424252D+05-1.898603142D+03 1.428134804D+01-4.776026950D-04 1.003097496D-07  
 -1.107859145D-11 4.990338200D-16 -1.614547674D+03-4.122943070D+01

SiH2 Gurvich,1991 pt1 p260. Fredin,1985. Dubois,1968.  
 2 g 3/01 SI 1.00H 2.00 0.00 0.00 0.00 0 30.1013800 273332.530  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.102  
 -2.063863564D+04 3.305862200D+02 2.099271145D+00 3.542539370D-03 3.378876670D-06  
 -5.383845620D-09 2.081191273D-12 3.011784298D+04 1.282333570D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10018.102  
 4.624039370D+06-1.143436110D+04 1.264880870D+01 9.114899500D-04-8.766611540D-07  
 1.646297357D-10-9.965090370D-15 1.072475101D+05-6.606078070D+01

SiH2Br2 Chase,1998 p481.  
 2 j12/76 SI 1.00H 2.00BR 2.00 0.00 0.00 0 189.9093800 -190372.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14272.222  
 1.651528003D+05-2.468145554D+03 1.608639427D+01-9.413840900D-03 1.407423872D-05  
 -9.240751450D-09 2.255641666D-12 -1.276482614D+04-5.945374320D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14272.222  
 5.665851440D+05-3.973919620D+03 1.567387912D+01-9.943802290D-04 2.084856022D-07  
 -2.299521351D-11 1.034736283D-15 -2.990690180D+03-6.190476520D+01

## Appendix D (continued)

SiH<sub>2</sub>CL<sub>2</sub> Chase, 1998 p823.  
 2 j12/76 SI 1.00H 2.00CL 2.00 0.00 0.00 0 101.0073800 -320494.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13384.948  
 1.894281754D+05-2.650960252D+03 1.549874174D+01-6.533130750D-03 9.306098260D-06  
 -5.639698670D-09 1.213664264D-12 -2.720912007D+04-6.006331649D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13384.948  
 5.400204580D+05-4.062337290D+03 1.573118788D+01-1.015038389D-03 2.127060243D-07  
 -2.345079226D-11 1.054871984D-15 -1.823098225D+04-6.544540499D+01

SiH<sub>2</sub>F<sub>2</sub> Chase, 1998 p1108.  
 2 j 6/76 SI 1.00H 2.00F 2.00 0.00 0.00 0 68.0981864 -790776.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11988.206  
 1.272188427D+05-1.241724310D+03 4.899435890D+00 2.123882008D-02-2.725708700D-05  
 1.860857446D-08-5.226604330D-12 -8.980466920D+04-5.111815500D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11988.206  
 4.726534080D+05-4.388517690D+03 1.596032597D+01-1.102993658D-03 2.315838331D-07  
 -2.556974559D-11 1.151499711D-15 -7.316184460D+04-7.098989270D+01

SiH<sub>2</sub>I<sub>2</sub> Chase, 1998 p1313.  
 2 j12/76 SI 1.00H 2.00I 2.00 0.00 0.00 0 283.9103200 -38074.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14917.266  
 1.539963319D+05-2.414436989D+03 1.684409354D+01-1.212037580D-02 1.808453226D-05  
 -1.207740133D-08 3.040799276D-12 5.073073250D+03-6.098720820D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14917.266  
 5.942390830D+05-3.924814480D+03 1.563850289D+01-9.805706340D-04 2.054871384D-07  
 -2.265587199D-11 1.019168663D-15 1.513627352D+04-5.940812520D+01

SiH<sub>3</sub> Gurvich, 1991 pt1 p261 pt2 p236.  
 2 g 3/99 SI 1.00H 3.00 0.00 0.00 0.00 0 31.1093200 204357.366  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10276.989  
 4.341142820D+03 2.277185085D+02 6.508250350D-01 1.221438558D-02-4.347604270D-06  
 -1.774916828D-09 1.184191367D-12 2.259993826D+04 1.968347482D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10276.989  
 6.056321220D+05-4.721254060D+03 1.329129523D+01-1.256824868D-03 2.688285940D-07  
 -3.010741582D-11 1.370945857D-15 4.974420640D+04-6.140503100D+01

SiH<sub>3</sub>Br Chase, 1998 p439.  
 2 j12/76 SI 1.00H 3.00BR 1.00 0.00 0.00 0 111.0133200 -78241.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11769.378  
 1.521065525D+05-1.987744479D+03 1.131460743D+01-1.806099407D-03 7.769262470D-06  
 -6.233478170D-09 1.585331846D-12 -9.248868880D+02-3.846463690D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11769.378  
 9.279285780D+05-5.917935790D+03 1.699209298D+01-1.487507364D-03 3.123451161D-07  
 -3.449071470D-11 1.553431675D-15 2.241560128D+04-7.948611590D+01

SiH<sub>3</sub>CL Chase, 1998 p764.  
 2 j12/76 SI 1.00H 3.00CL 1.00 0.00 0.00 0 66.5623200 -141838.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11440.706  
 1.633388301D+05-2.030302118D+03 1.068016138D+01 4.942370140D-04 4.305174760D-06  
 -3.748327270D-09 8.893504210D-13 -8.180714980D+03-3.688956824D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11440.706  
 9.087780940D+05-5.958949560D+03 1.702076016D+01-1.498450667D-03 3.146813781D-07  
 -3.475168460D-11 1.565281681D-15 1.493793206D+04-8.127277864D+01

SiH<sub>3</sub>F Chase, 1998 p1058.  
 2 j 6/76 SI 1.00H 3.00F 1.00 0.00 0.00 0 50.1077232 -376560.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10931.622  
 1.267836290D+05-1.177593516D+03 4.499188960D+00 1.658543011D-02-1.678598921D-05  
 1.019153931D-08-2.803920232D-12 -4.010392970D+04-4.481080920D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10931.622  
 8.624313170D+05-6.103370570D+03 1.712733597D+01-1.540724131D-03 3.239628720D-07  
 -3.581056890D-11 1.614151380D-15 -1.261487616D+04-8.399227210D+01

SiH<sub>3</sub>I Chase, 1998 p1342.  
 2 j12/76 SI 1.00H 3.00I 1.00 0.00 0.00 0 158.0137900 -2092.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12078.229  
 1.459384799D+05-1.982982746D+03 1.196516737D+01-3.937505950D-03 1.087991733D-05  
 -8.433135920D-09 2.196078188D-12 8.063208310D+03-4.064553320D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12078.229  
 9.361149180D+05-5.859720290D+03 1.695376698D+01-1.473497130D-03 3.094475885D-07  
 -3.417462470D-11 1.539334807D-15 3.127499231D+04-7.801700080D+01

## Appendix D (continued)

SiH<sub>4</sub> Silane, Gurvich, 1991 pt1 p263 pt 2 p237.  
 2 tpsis91 SI 1.00H 4.00 0.00 0.00 0.00 0 32.1172600 34700.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10535.001  
 7.872993290D+04-5.526087050D+02 2.498944303D+00 1.442118274D-02-8.467107310D-06  
 2.726164641D-09-5.436754370D-13 6.269669060D+03 4.965461830D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10535.001  
 1.290378740D+06-7.813399780D+03 1.828851664D+01-1.975620946D-03 4.156502150D-07  
 -4.596745610D-11 2.072777131D-15 4.766887950D+04-9.801697460D+01

SiI Gurvich, 1991 pt1 p284 pt2 p253.  
 2 tpsis91 SI 1.00I 1.00 0.00 0.00 0.00 0 154.9899700 262953.420  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9941.120  
 9.492081340D+04-1.573960062D+03 1.237908109D+01-1.593864820D-02 1.692049005D-05  
 -9.215558320D-09 2.046186848D-12 3.779735670D+04-4.066407850D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9941.120  
 8.529402790D+05-2.442039471D+03 7.722977520D+00-1.985601243D-03 6.542866630D-07  
 -9.494158290D-11 4.890041370D-15 4.578160940D+04-1.733975081D+01

SiI<sub>2</sub> Chase, 1998 p1432.  
 2 j12/76 SI 1.00I 2.00 0.00 0.00 0.00 0 281.8944400 92466.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13792.515  
 1.163352403D+04-4.514482170D+02 8.707978130D+00-3.580664930D-03 4.253714430D-06  
 -2.673478266D-09 6.891558980D-13 1.126247142D+04-1.155818335D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13792.515  
 1.002168907D+04 1.433017148D+01 6.701330550D+00 3.960769900D-04-2.073866165D-07  
 4.553457100D-11-3.016798280D-15 9.007368100D+03 2.887336913D-01

SiN Gurvich, 1991 pt1 p295 pt2 p261.  
 2 g 5/99 SI 1.00N 1.00 0.00 0.00 0.00 0 42.0922000 403668.437  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8736.137  
 -1.464672152D+04 1.374993497D+02 3.678508580D+00-6.158499200D-03 2.309417067D-05  
 -2.294461481D-08 7.395665680D-12 4.673212990D+04 6.494564115D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8736.137  
 -2.932685132D+06 5.853688590D+03 1.321451677D+00 1.258329284D-03-3.773886360D-07  
 -6.887761040D-11-4.189842590D-15 6.527148810D+03 2.553145732D+01

SiO Gurvich, 1991 pt1 p247 pt2 p227  
 2 tpsis91 SI 1.00O 1.00 0.00 0.00 0.00 0 44.0849000 -98842.418  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8715.105  
 -4.722771050D+04 8.063137640D+02-1.636976133D+00 1.454275546D-02-1.723202046D-05  
 1.042397340D-08-2.559365273D-12 -1.666585903D+04 3.355795700D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8715.105  
 -1.765134162D+05-3.199177090D+01 4.477441930D+00 4.591764710D-06 3.558143150D-08  
 -1.327012559D-11 1.613253297D-15 -1.350842360D+04-8.386957330D-01

SiO<sub>2</sub> Gurvich, 1991 pt1 p256 pt2 p233.  
 2 tpsis91 SI 1.00O 2.00 0.00 0.00 0.00 0 60.0843000 -322073.477  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10542.523  
 -3.362948780D+04 4.734078920D+02 2.309770671D-01 1.850230806D-02-2.242786671D-05  
 1.364981554D-08-3.351935030D-12 -4.226487490D+04 2.295803206D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10542.523  
 -1.464031193D+05-6.261441060D+02 7.964563710D+00-1.854119096D-04 4.095214670D-08  
 -4.697206760D-12 2.178054280D-16 -3.791834770D+04-2.045285414D+01

SiS Gurvich, 1991 pt1 p290 pt2 p258.  
 2 tpsis91 SI 1.00S 1.00 0.00 0.00 0.00 0 60.1505000 108194.407  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8932.107  
 3.599449290D+04-4.239723300D+02 4.654014420D+00 1.588470782D-03-3.310254360D-06  
 2.706096479D-09-8.113517820D-13 1.411515571D+04-1.183201858D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8932.107  
 -2.102323897D+06 6.228836180D+03-3.004120882D+00 4.495499930D-03-1.368821364D-06  
 1.998097253D-10-9.882035800D-15 -2.795538166D+04 5.405828786D+01

SiS<sub>2</sub> Gurvich, 1991 pt1 p294 pt2 p260.  
 2 tpsis91 SI 1.00S 2.00 0.00 0.00 0.00 0 92.2155000 7022.717  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12203.217  
 4.397745660D+04-7.430013120D+02 7.941588360D+00 2.038083730D-03-4.646337600D-06  
 3.848014360D-09-1.157260149D-12 2.801077853D+03-1.736888325D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12203.217  
 -1.266489071D+05-9.774235220D+01 7.572803680D+00-2.905413928D-05 6.405587840D-09  
 -7.329273340D-13 3.389819780D-17 -1.244672263D+03-1.352710463D+01

## Appendix D (continued)

Si2 Gurvich,1991 pt1 p240 pt2 p225.  
 2 tpis91 SI 2.00 0.00 0.00 0.00 0.00 0 56.1710000 580195.524  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10296.124  
 1.237596221D+04-1.024904376D+02 4.354848520D+00 1.281063335D-03-2.531991623D-06  
 2.265694244D-09-7.001290140D-13 6.906942850D+04 3.251125200D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10296.124  
 1.370060657D+06-4.207060040D+03 9.337432890D+00-2.749217168D-03 9.586345960D-07  
 -1.372449748D-10 6.765028100D-15 9.510884540D+04-3.168385190D+01

Si2C Gurvich,1991 pt1 p304 pt2 p267.  
 2 tpis91 SI 2.00C 1.00 0.00 0.00 0.00 0 68.1817000 554093.904  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11582.346  
 -4.553366200D+03 1.314796415D+02 2.469106923D+00 1.276520680D-02-1.656910776D-05  
 1.065289663D-08-2.739192976D-12 6.470049920D+04 1.468838980D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11582.346  
 -1.253829442D+05-3.414277790D+02 7.254365330D+00-1.017635503D-04 2.250902158D-08  
 -2.584074852D-12 1.198884876D-16 6.608009380D+04-1.146216579D+01

Si2F6 Lyman,2001.  
 2 g 6/01 SI 2.00F 6.00 0.00 0.00 0.00 0 170.1614192 -2383290.080  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26694.292  
 1.580767450D+04-2.975292881D+02 7.512591500D+00 4.552796230D-02-6.421876840D-05  
 4.357408730D-08-1.166762282D-11 -2.886707444D+05-7.721784770D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26694.292  
 -9.186303140D+05 1.573948683D+02 2.141256129D+01-2.681898667D-04 7.212280110D-08  
 -9.184252660D-12 4.537238360D-16 -2.966176753D+05-7.849022470D+01

Si2N Chase,1998 p1611.  
 2 j 3/67 SI 2.00N 1.00 0.00 0.00 0.00 0 70.1777000 397480.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11822.188  
 2.318271938D+04-3.674843790D+02 5.409658600D+00 8.176389400D-03-1.220312934D-05  
 8.580609100D-09-2.354927059D-12 4.809278030D+04-3.042205654D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11822.188  
 -2.805026986D+05 2.502366876D+02 7.092456100D+00 2.853120795D-04-9.792101810D-08  
 1.552154244D-11-8.036260450D-16 4.342014790D+04-1.009570910D+01

Si3 Gurvich,1991 pt1 p246 pt2 p226.  
 2 g 7/95 SI 3.00 0.00 0.00 0.00 0.00 0 84.2565000 627867.381  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12519.793  
 -1.114208177D+04 1.575785843D+02 2.486135003D+00 1.631637255D-02-2.208240021D-05  
 1.372008287D-08-3.262330700D-12 7.328253850D+04 1.588081347D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12519.793  
 -1.699395561D+06 4.697815380D+03 2.618198124D+00 1.959082075D-03-2.581160603D-07  
 6.103444860D-12 6.086309240D-16 4.277916810D+04 2.586540384D+01

Sn Hf:Cox,1989 Moore,1971. Gordon,1999.  
 3 g 7/97 SN 1.00 0.00 0.00 0.00 0.00 0 118.7100000 301200.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6214.713  
 -1.248692263D+05 1.618841190D+03-4.602397350D+00 1.045433308D-02 2.998265550D-06  
 -1.068699386D-08 4.323421310D-12 2.748364008D+04 4.805067230D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6214.713  
 -5.145695640D+06 1.140575108D+04-4.179632060D+00 2.236390679D-03-3.603219770D-07  
 2.440237836D-11-2.937628285D-16 -4.215013570D+04 5.981450930D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6214.713  
 -1.119787114D+09 6.427046040D+05-1.378615913D+02 1.453867222D-02-7.109586030D-07  
 1.501409263D-11-8.940758657D-17 -5.111296870D+06 1.245625545D+03

Sn+ Moore,1971. Gordon,1999.  
 3 g 7/97 SN 1.00E -1.00 0.00 0.00 0.00 0 118.7094514 1015949.928  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 -5.571297780D+03 1.222323189D+02 1.566361415D+00 3.397061410D-03-6.312922290D-06  
 5.585452080D-09-1.689021340D-12 1.209024120D+05 1.162634765D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 4.622916850D+06-1.185958712D+04 1.237026473D+01-2.773624217D-03 3.098513490D-07  
 -5.362951440D-12-8.663474691D-16 1.994322977D+05-6.837108280D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6197.428  
 1.913728057D+08-1.145730242D+05 3.070294184D+01-3.387878800D-03 1.966377351D-07  
 -4.388396290D-12 2.057062343D-17 1.031631149D+06-2.370157923D+02



## Appendix D (continued)

Sn- Hotop,1985. Gordon,1999.

3 g 9/97 SN 1.00E 1.00 0.00 0.00 0.00 0 118.7105486 179495.949  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6490.449  
 2.722796000D+05-3.369935800D+03 1.743906405D+01-2.810527618D-02 2.790684767D-05  
 -1.442400675D-08 3.070159757D-12 3.753227750D+04-8.007856970D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6490.449  
 -6.447713220D+04 7.430555100D+02 1.921380256D+00 2.361623997D-04-5.280668360D-08  
 6.102339380D-12-2.843422486D-16 1.645739414D+04 1.265436865D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6490.449  
 -1.314284778D+06 8.972354270D+02 2.302354538D+00 2.246840970D-05-1.392571963D-09  
 4.468904450D-14-5.811846560D-19 1.428800599D+04 1.004933765D+01

SnBr Gurvich,1991 pt1 p378 pt2 p321.

2 tpis91 SN 1.00BR 1.00 0.00 0.00 0.00 0 198.6140000 75644.020  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9986.120  
 2.564193542D+04-5.259122330D+02 7.687410690D+00-9.654205420D-03 1.482863248D-05  
 -9.942236980D-09 2.475051091D-12 1.020483889D+04-1.126550396D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9986.120  
 1.815578541D+06-6.728264580D+03 1.332464516D+01-4.608102300D-03 1.236439537D-06  
 -1.528863587D-10 6.971513500D-15 4.925583090D+04-5.640962780D+01

SnBr2 Gurvich,1991 pt1 p380 pt2 p323.

2 tpis91 SN 1.00BR 2.00 0.00 0.00 0.00 0 278.5180000 -118974.592  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14595.408  
 -4.995753060D+03-1.366498896D+02 7.543563850D+00-1.181772507D-03 1.442445852D-06  
 -9.254217260D-10 2.423731634D-13 -1.575506969D+04-3.595584020D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14595.408  
 -1.940894091D+04-2.335607932D+00 7.001969260D+00-8.622241870D-07 2.039869794D-10  
 -2.464780359D-14 1.189850894D-18 -1.644828122D+04-4.349354750D-01

SnBr3 Gurvich,1991 pt1 p381 pt2 p324.

2 tpis91 SN 1.00BR 3.00 0.00 0.00 0.00 0 358.4220000 -158716.446  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19280.454  
 -8.050416470D+03-2.897962523D+02 1.114443355D+01-2.475383807D-03 3.010051350D-06  
 -1.925695320D-09 5.032605090D-13 -2.070066649D+04-1.895965383D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19280.454  
 -3.893004530D+04-4.990844170D+00 1.000418437D+01-1.824996910D-06 4.305646660D-10  
 -5.191887930D-14 2.502455595D-18 -2.217299473D+04-1.229854098D+01

SnBr4 Gurvich,1991 pt1 p384 pt2 p326.

2 tpis91 SN 1.00BR 4.00 0.00 0.00 0.00 0 438.3260000 -324216.982  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 25043.018  
 -5.832840920D+03-4.270198470D+02 1.467466525D+01-3.604263230D-03 4.366686290D-06  
 -2.785875130D-09 7.265087870D-13 -4.082916450D+04-3.447104360D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 25043.018  
 -5.176812920D+04-7.426126950D+00 1.300619502D+01-2.692587978D-06 6.336759800D-10  
 -7.627087190D-14 3.671112000D-18 -4.300166340D+04-2.471455118D+01

SnCL Gurvich,1991 pt1 p370 pt2 p315.

2 tpis91 SN 1.00CL 1.00 0.00 0.00 0.00 0 154.1630000 34658.816  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9644.116  
 3.351549730D+04-6.832208620D+02 8.393917730D+00-1.164434373D-02 1.812159499D-05  
 -1.261999170D-08 3.295213470D-12 6.051790890D+03-1.667834578D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9644.116  
 7.741605680D+05-3.602048480D+03 9.749059820D+00-2.596198909D-03 6.367712160D-07  
 -6.754295570D-11 2.484167602D-15 2.442447662D+04-3.225454098D+01

SnCL2 Gurvich,1991 pt1 p373 pt2 p317.

2 tpis91 SN 1.00CL 2.00 0.00 0.00 0.00 0 189.6160000 -202648.283  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13681.717  
 9.524665900D+03-4.329845640D+02 8.644720280D+00-3.458409610D-03 4.117852030D-06  
 -2.592639269D-09 6.692363600D-13 -2.432921127D+04-1.299143851D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13681.717  
 -3.903588490D+04-7.947962680D+00 7.006487620D+00-2.776594714D-06 6.461341420D-10  
 -7.119067400D-15 3.688131180D-18 -2.654529653D+04-3.368081174D+00

SnCL3 Gurvich,1991 pt1 p374 pt2 p318.

2 tpis91 SN 1.00CL 3.00 0.00 0.00 0.00 0 225.0690000 -292372.455  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17554.045  
 1.760076813D+04-8.142805480D+02 1.306326984D+01-6.395596190D-03 7.574624570D-06  
 -4.749711460D-09 1.222182656D-12 -3.413430960D+04-3.457679670D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17554.045  
 -7.482966400D+04-1.528523914D+01 1.001240305D+01-5.285581240D-06 1.226095111D-09  
 -1.459895108D-13 6.968879780D-18 -3.830878270D+04-1.663063137D+01

## Appendix D (continued)

SnCL4                    Gurvich,1991 pt1 p376 pt2 p320.

2 tps91 SN	1.00CL	4.00	0.00	0.00	0.00	0.00	0	260.5220000	-478465.969
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.245967870D+04	-1.280574318D+03	1.768445328D+01	-9.574779520D-03	1.115620323D-05					
-6.907229270D-09	1.759652856D-12							-5.504009040D+04	-5.827352999D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.078336862D+05	-2.554305872D+01	1.302040391D+01	-8.595125900D-06	1.976570888D-09					
-2.337929994D-13	1.110287624D-17							-6.163562030D+04	-3.072702622D+01

SnF                    Gurvich,1991 pt1 p365 pt2 p310.

2 tps91 SN	1.00F	1.00	0.00	0.00	0.00	0	137.7084032	-95017.090	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.098503520D+04	-9.860306290D+02	8.994731210D+00	-1.223012156D-02	1.840583578D-05					
-1.267926607D-08	3.291331020D-12							-7.882614480D+03	-2.221921734D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.589715476D+04	-1.484478214D+03	7.378518930D+00	-1.324244440D-03	2.847634043D-07					
-2.360371345D-11	6.116783710D-16							-4.776688970D+03	-1.681202516D+01

SnF2                    Gurvich,1991 pt1 p368 pt2 p312.

2 tps91 SN	1.00F	2.00	0.00	0.00	0.00	0	156.7068064	-510956.951	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.042391850D+04	-1.137505955D+03	1.008659352D+01	-4.722855930D-03	4.135702920D-06					
-1.921143972D-09	3.640760280D-13							-5.756670820D+04	-2.571566624D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.027758772D+05	-4.451751620D+01	7.033268760D+00	-1.329882797D-05	2.934271938D-09					
-3.358415920D-13	1.553358669D-17							-6.362125880D+04	-6.810084520D+00

SnF3                    Gurvich,1991 pt1 p369 pt2 p313.

2 tps91 SN	1.00F	3.00	0.00	0.00	0.00	0	175.7052096	-646630.479	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.095555529D+05	-1.950557979D+03	1.541407832D+01	-8.546518770D-03	7.800551820D-06					
-3.825942220D-09	7.787747760D-13							-7.056794920D+04	-5.494639480D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.829319689D+05	-7.557358680D+01	1.005671455D+01	-2.275132668D-05	5.034695820D-09					
-5.776530960D-13	2.677214170D-17							-8.091897590D+04	-2.191673972D+01

SnF4                    Gurvich,1991 pt1 p369 pt2 p314.

2 tps91 SN	1.00F	4.00	0.00	0.00	0.00	0	194.7036128	-1024766.717	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.390441119D+05	-2.168784371D+03	1.691802917D+01	-2.318608529D-03	-2.045847976D-06					
3.430087900D-09	-1.289228860D-12							-1.153563396D+05	-6.370604750D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.635692764D+05	-1.445469969D+02	1.310690681D+01	-4.237755790D-05	9.286871950D-09					
-1.057062694D-12	4.867108680D-17							-1.271539967D+05	-3.803921900D+01

SnI                    Gurvich,1991 pt1 p384 pt2 p327.

2 tps91 SN	1.00I	1.00	0.00	0.00	0.00	0	245.6144700	172725.022	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.670212235D+04	-5.006026350D+02	7.490673150D+00	-8.746346550D-03	1.289688397D-05					
-8.211344930D-09	1.936120475D-12							2.177249172D+04	-9.354806850D+00
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.554991850D+04	-1.530457453D+03	7.932601390D+00	-2.108885464D-03	7.809803600D-07					
-1.348104887D-10	8.207184700D-15							2.744864953D+04	-1.626822892D+01

SnI2                    Gurvich,1991 pt1 p387 pt2 p329.

2 tps91 SN	1.00I	2.00	0.00	0.00	0.00	0	372.5189400	-8066.737	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.739254890D+03	-9.435024450D+01	7.377956660D+00	-8.258348940D-04	1.011687040D-06					
-6.508451600D-10	1.708186600D-13							-2.622644500D+03	-9.605814960D-01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.559453390D+04	-1.594789414D+00	7.001351160D+00	-5.935324240D-07	1.407432564D-10					
-1.703457321D-14	8.233611710D-19							-3.100608319D+03	1.235038509D+00

SnI3                    Gurvich,1991 pt1 p388 pt2 p330.

2 tps91 SN	1.00I	3.00	0.00	0.00	0.00	0	499.4234100	-8017.540	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.069978099D+04	-1.387693540D+02	1.055637633D+01	-1.216435658D-03	1.490873499D-06					
-9.594499630D-10	2.518810438D-13							-3.314229880D+03	-1.249558209D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.517534870D+04	-2.348282890D+00	1.000199130D+01	-8.752764840D-07	2.076464980D-10					
-2.514060336D-14	1.215482266D-18							-4.017055610D+03	-9.263908460D+00

## Appendix D (continued)

SnI4                      Gurvich,1991 pt1 p391 pt2 p332.

2 tps91 SN	1.00I	4.00	0.00	0.00	0.00	0.00	0	626.3278800	-118854.043
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.283146793D+04	-1.459885093D+02	1.358634885D+01	-1.283554646D-03	1.574557147D-06					
-1.013990168D-09	2.663370430D-13		-1.751178045D+04	-2.367973168D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.801840706D+04	-2.474699366D+00	1.300210215D+01	-9.250962340D-07	2.196515817D-10					
-2.661071614D-14	1.287167546D-18		-1.825083832D+04	-2.027484281D+01					

SnO                      Gurvich,1991 pt1 p359 pt2 p307.

2 tps91 SN	1.00O	1.00	0.00	0.00	0.00	0	134.7094000	21911.054	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.547788022D+04	-2.293583066D+02	3.421593530D+00	4.713300040D-03	-7.365971320D-06					
5.379738870D-09	-1.519277855D-12		2.853047679D+03	6.673965270D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.55595548D+06	7.870053500D+03	-5.439768730D+00	6.307819180D-03	-2.068871370D-06					
3.307074880D-10	-1.848169716D-14		-4.841663910D+04	7.175952460D+01					

SnO2                      Gurvich,1991 pt1 p364 pt2 p309.

2 tps91 SN	1.00O	2.00	0.00	0.00	0.00	0	150.7088000	11680.180	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.707674080D+04	-6.114568670D+02	6.117433910D+00	7.514014660D-03	-1.238371787D-05					
9.220915990D-09	-2.632417597D-12		2.981068066D+03	-8.144926410D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.573558926D+05	-1.427316788D+02	7.605700760D+00	-4.198008530D-05	9.218742430D-09					
-1.051372983D-12	4.849579270D-17		-5.234531870D+02	-1.428360169D+01					

SnS                      Gurvich,1991 pt1 p394 pt2 p334.

2 tps91 SN	1.00S	1.00	0.00	0.00	0.00	0	150.7750000	111099.012	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.724877813D+04	-4.924126380D+02	6.221654730D+00	-3.409406960D-03	3.984913680D-06					
-2.470702874D-09	6.339341460D-13		1.452495307D+04	-6.791285229D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.797985129D+06	6.141736320D+03	-4.019504880D+00	5.993829180D-03	-2.188735204D-06					
3.899542000D-10	-2.406563630D-14		-2.611349815D+04	6.256820705D+01					

SnS2                      Gurvich,1991 pt1 p397 pt2 p336.

2 tps91 SN	1.00S	2.00	0.00	0.00	0.00	0	182.8400000	149645.595	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.877145410D+04	-8.486953940D+02	1.042083990D+01	-5.686902670D-03	6.373829770D-06					
-3.825158100D-09	9.502480960D-13		2.006027952D+04	-2.723724769D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-6.764084050D+04	-1.970189679D+01	7.515333870D+00	-6.332559180D-06	1.434207625D-09					
-1.676383081D-13	7.886911900D-18		1.565053629D+04	-9.922744838D+00					

Sn2                      Gurvich,1991 pt1 p354 pt2 p305.

2 tps91 SN	2.00	0.00	0.00	0.00	0.00	0	237.4200000	421343.737	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.329666654D+05	1.639179787D+03	-1.902868972D+00	1.290431677D-02	-1.120542242D-05					
4.502993860D-09	-6.056237770D-13		4.097452710D+04	4.435408030D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.275783040D+06	1.236421656D+04	-8.438336170D+00	7.088056290D-03	-1.712012737D-06					
1.805262952D-10	-7.058656810D-15		-3.001418720D+04	1.005138538D+02					

Sr                      Hf:Gurvich,1996a. Moore,1971. Moore,1970a. Gordon,1999.

3 g 1/98 SR	1.00	0.00	0.00	0.00	0.00	0	87.6200000	160500.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.190649840D+00	-6.304437580D-02	2.500373027D+00	-1.115455943D-06	1.785248643D-09					
-1.456209589D-12	4.750132981D-16		1.855852648D+04	5.555772840D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.489414410D+07	-4.375335050D+04	5.137266280D+01	-2.592566025D-02	6.582990000D-06					
-6.949611800D-10	2.417779662D-14		2.977545522D+05	-3.454890770D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.562233720D+08	-6.093193220D+05	2.109096848D+02	-3.010063957D-02	2.178021676D-06					
-7.824003460D-11	1.109909620D-15		4.579268340D+06	-1.752716908D+03					

Sr+                      Moore,1971. Gordon,1999.

3 g 1/98 SR	1.00E	-1.00	0.00	0.00	0.00	0	87.6194514	716166.328	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.127287678D+01	-1.346951870D-01	2.500651495D+00	-1.635163061D-06	2.249493149D-09					
-1.610827539D-12	4.698612333D-16		8.538981180D+04	6.247259240D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.145095058D+06	-9.514756890D+03	1.350086948D+01	-6.059717120D-03	1.594068746D-06					
-1.718800946D-10	6.322256169D-15		1.457991907D+05	-7.236416930D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
9.016769220D+08	-6.244641660D+05	1.695763594D+02	-2.154835606D-02	1.462482744D-06					
-4.930465390D-11	6.505705019D-16		4.966238870D+06	-1.431844579D+03					

## Appendix D (continued)

SrBr Gurvich,1996a pt1 p522 pt2 p402.

3 tps96 SR	1.00BR	1.00	0.00	0.00	0.00	0.00	0	167.5240000	-63917.678
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.549812420D+02	-7.359532010D+01	4.828035810D+00	-7.160584650D-04	1.028527433D-06					
-6.888370720D-10	1.880257878D-13		-8.686168450D+03	4.151153090D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.009976114D+06	-9.193192240D+03	1.526033745D+01	-6.009253950D-03	1.692611858D-06					
-2.039438429D-10	8.807775840D-15		4.922806130D+04	-7.068253830D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.274974243D+08	-1.566004653D+05	4.234598410D+01	-3.477076740D-03	1.358747452D-07					
-2.623018618D-12	1.969298231D-17		1.221445664D+06	-3.265840740D+02					

SrBr2 Gurvich,1996a pt1 p524 pt2 p404.

2 tps96 SR	1.00BR	2.00	0.00	0.00	0.00	0	247.4280000	-406725.851	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.632458660D+03	-7.244938640D+01	7.800217160D+00	-6.772125310D-04	8.537780240D-07					
-5.632331740D-10	1.510568795D-13		-5.082238330D+04	-5.285074760D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.186173059D+04	-1.404383013D+00	7.501215570D+00	-5.415983190D-07	1.296969275D-10					
-1.580911652D-14	7.681582270D-19		-5.118575210D+04	-3.552037110D+00					

SrCL Gurvich,1996a pt1 p515 pt2 p398.

3 tps96 SR	1.00CL	1.00	0.00	0.00	0.00	0	123.0730000	-127867.882	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.555346320D+03	-1.729385697D+02	5.213451020D+00	-1.542910668D-03	2.025835568D-06					
-1.327076633D-09	3.547175960D-13		-1.588288066D+04	4.818144784D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.070217324D+06	-6.199891730D+03	1.150315072D+01	-3.675685460D-03	9.461732350D-07					
-9.203765750D-11	2.707242192D-15		2.271471632D+04	-4.561058514D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.382269500D+08	-9.659524410D+04	2.600419230D+01	-1.405193291D-03	2.007238545D-08					
7.119698480D-13	-2.001316762D-17		7.447979070D+05	-1.876849167D+02					

SrCL+ Gurvich,1996a pt1 p516 pt2 p399.

3 g 8/98 SR	1.00CL	1.00E	-1.00	0.00	0.00	0	123.0724514	408112.162	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.689043529D+03	-1.749284676D+02	5.065328640D+00	-9.857327840D-04	1.071655138D-06					
-5.988127130D-10	1.395650932D-13		4.861190260D+04	2.492001711D-01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.132475783D+04	-4.057948270D+00	4.503149390D+00	3.826202380D-05	2.676951510D-09					
5.667610500D-14	1.613288103D-18		4.769326030D+04	3.637722496D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.041313813D+04	-7.208302400D+00	4.501589780D+00	3.937923600D-05	2.394465390D-09					
9.062292570D-14	4.723672450D-21		4.772357520D+04	3.647375336D+00					

SrCL2 Gurvich,1996a pt1 p520 pt2 p401.

2 tps96 SR	1.00CL	2.00	0.00	0.00	0.00	0	158.5260000	-484813.902	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.913170011D+03	-2.681156951D+02	8.081334300D+00	-2.393329295D-03	2.976397494D-06					
-1.943902862D-09	5.174307710D-13		-5.910111850D+04	-8.457827543D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.592716099D+04	-5.263785850D+00	7.004475240D+00	-1.970397814D-06	4.679671200D-10					
-5.670215880D-14	2.742892387D-18		-6.045399530D+04	-2.192202775D+00					

SrF Gurvich,1996a pt1 p507 pt2 p394.

3 tps96 SR	1.00F	1.00	0.00	0.00	0.00	0	106.6184032	-303552.788	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.725008615D+04	-4.850019720D+02	6.112697200D+00	-3.008469209D-03	3.368465800D-06					
-1.987813072D-09	4.884161090D-13		-3.536890390D+04	-6.683739180D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.702340490D+05	-2.589818770D+03	7.200264220D+00	-1.173446296D-03	1.996165066D-07					
1.103842667D-11	2.343183859D-15		-2.133671699D+04	-1.667390309D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.448093370D+07	2.208058158D+04	-5.125719860D+00	2.209099383D-03	-1.551627196D-07					
5.125524390D-12	-6.680071600D-17		-2.048593542D+05	7.995585500D+01					

SrF+ Gurvich,1996a pt1 p511 pt2 p395.

3 g 8/98 SR	1.00F	1.00E	-1.00	0.00	0.00	0	106.6178546	209468.312	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.009624200D+04	-5.944946080D+02	6.182330330D+00	-2.716159750D-03	2.641369127D-06					
-1.383123292D-09	3.052935853D-13		2.697149351D+04	-8.313659450D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.752082060D+04	-2.526802345D+01	4.519295280D+00	2.556426750D-05	3.382541830D-09					
-1.511394636D-13	9.537491180D-18		2.383861417D+04	1.892197325D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.403608095D+03	-3.242568700D+01	4.507124800D+00	3.261116540D-05	1.672393446D-09					
5.130259820D-14	2.102366585D-20		2.392692006D+04	1.974517090D+00					

## Appendix D (continued)

SrF2                      Gurvich,1996a pt1 p514 pt2 p397.

2	tpis96	SR	1.00F	2.00	0.00	0.00	0.00	0	125.6168064	-784793.795
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
4.170759650D+04	-8.500132410D+02	1.002806064D+01	-6.098485190D-03	7.056261330D-06						
-4.359374310D-09	1.111308310D-12									
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13269.601
-6.126265430D+04	-1.964060822D+01	7.015557750D+00	-6.512526780D-06	1.490473613D-09						
-1.756437040D-13	8.317093850D-18									

SrH                      Gurvich,1996a pt1 p499 pt2 p388.

2	tpis96	SR	1.00H	1.00	0.00	0.00	0.00	0	88.6279400	219227.105
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.317796890D+04	7.676429700D+02	-1.594398638D+00	1.500711077D-02	-1.826296898D-05						
1.136757659D-08	-2.855588359D-12									
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	8723.105
-2.269825428D+05	1.345209458D+03	1.152194421D+00	3.109555289D-03	-1.188080968D-06						
2.073091147D-10	-1.300839287D-14									

SrI                      Gurvich,1996a pt1 p526 pt2 p405.

3	tpis96	SR	1.00I	1.00	0.00	0.00	0.00	0	214.5244700	-7851.676
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.467498501D+03	-2.535495809D+01	4.603298480D+00	-1.613676212D-04	2.694296409D-07						
-1.564795762D-10	3.826482280D-14									
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10283.124
2.201136857D+06	-7.082230700D+03	1.332597928D+01	-5.305864420D-03	1.636071150D-06						
-2.205540591D-10	1.078496824D-14									
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	10283.124
1.557303348D+08	-1.150787674D+05	3.550520760D+01	-3.375329300D-03	1.695651221D-07						
-4.438653930D-12	4.852777450D-17									

SrI2                      Gurvich,1996a pt1 p528 pt2 p407.

2	tpis96	SR	1.00I	2.00	0.00	0.00	0.00	0	341.4289400	-278218.842
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.391849690D+03	-3.757267350D+01	7.656993500D+00	-3.561721300D-04	4.508689010D-07						
-2.983230473D-10	8.018658660D-14									
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	16701.658
-8.090381920D+03	-7.348263230D-01	7.500640060D+00	-2.863515042D-07	6.876556970D-11						
-8.398807360D-15	4.086968160D-19									

SrO                      Gurvich,1996a pt1 p495 pt2 p384.

3	tpis96	SR	1.00O	1.00	0.00	0.00	0.00	0	103.6194000	-14207.691
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
4.224891670D+04	-5.913517870D+02	5.964363000D+00	-2.105712736D-03	2.028373972D-06						
-1.197885492D-09	3.466289920D-13									
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	9040.109
-5.172933050D+07	1.510821000D+05	-1.614513515D+02	8.516051790D-02	-2.091669402D-05						
2.452307103D-09	-1.108841292D-13									
6000.000	20000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
1.988729112D+08	-9.438733680D+04	2.862378041D+01	-2.923338947D-03	1.808436182D-07						
-5.719087480D-12	7.320935570D-17									

SrO+                      Gurvich,1996a pt1 p497 pt2 p386. Partridge,1986.

3	g	8/98	SR	1.00O	1.00E	-1.00	0.00	0.00	0	103.6188514	630053.722
298.150	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0	
4.618674160D+04	-4.604560920D+02	5.605360720D+00	-1.511707524D-03	1.328692506D-06							
-6.244610540D-10	1.274632229D-13										
1000.000	6000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0	
1.035147885D+06	-3.339081120D+03	8.520055290D+00	-2.340803237D-03	7.338594440D-07							
-1.031868417D-10	5.087079240D-15										
6000.000	20000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0	
-6.910421610D+07	1.253686165D+04	9.522159370D+00	-1.279343636D-03	8.998760920D-08							
-2.931863956D-12	3.752244570D-17										

SrOH                      Gurvich,1996a pt1 p502 pt2 p390.

2	tpis96	SR	1.00O	1.00H	1.00	0.00	0.00	0	104.6273400	-194085.726
200.000	1000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
4.640006560D+04	-9.938685540D+02	9.784948960D+00	-5.774377620D-03	5.126164110D-06						
-1.833418356D-09	1.926013410D-13									
1000.000	6000.0007	-2.0	-1.0	0.0	0.0	1.0	2.0	3.0	4.0	0.0
2.545648379D+06	-7.416195980D+03	1.381956204D+01	-3.096481934D-03	7.723894210D-07						
-7.921280320D-11	2.740829111D-15									

## Appendix D (continued)

SrOH+ Gurvich,1996a pt1 p503 pt2 p391.

2 tps96 SR	1.000	1.00H	1.00E	-1.00	0.00	0	104.6267914	310169.605
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.857366940D+04	-9.030242330D+02	9.451103250D+00	-5.042516280D-03	4.190101890D-06				
-1.196920603D-09	1.606318743D-14		3.995067720D+04	-2.601486110D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.679695660D+05	-2.340609538D+03	7.976829750D+00	1.023752569D-04	-6.286032330D-08				
1.024851502D-11	-5.723683920D-16		5.073157720D+04	-2.027046917D+01				

Sr(OH)2 Gurvich,1996a pt1 p506 pt2 p393.

2 tps96 SR	1.000	2.00H	2.00	0.00	0.00	0	121.6346800	-596694.573
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.205090300D+04	-1.789465226D+03	1.729429139D+01	-1.169280781D-02	1.106702894D-05				
-4.490146090D-09	6.603997460D-13		-6.605394040D+04	-6.388681220D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.750013518D+06	-4.681601500D+03	1.395548402D+01	2.035019560D-04	-1.253496115D-07				
2.044549432D-11	-3.142004855D-15		-4.427170240D+04	-5.051456850D+01				

SrS Gurvich,1996a pt1 p529 pt2 p409.

2 tps96 SR	1.00S	1.00	0.00	0.00	0.00	0	119.6850000	104351.315
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.256440807D+04	-3.150436559D+02	5.721722510D+00	-2.630479718D-03	3.384699750D-06				
-2.296256846D-09	6.512086680D-13		1.277295160D+04	-3.693874943D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.379432947D+07	3.921331580D+04	-3.602866380D+01	1.818513386D-02	-3.275858160D-06				
2.324312746D-10	-3.614555700D-15		-2.410246179D+05	2.991679642D+02				

Sr2 Gurvich,1996a pt1 p491 pt2 p382.

2 tps96 SR	2.00	0.00	0.00	0.00	0.00	0	175.2400000	307570.337
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.108859753D+05	5.927604010D+02	8.439688550D+00	-2.652801112D-02	4.435825970D-05				
-3.399915490D-08	9.965546680D-12		3.157615033D+04	-7.033966650D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.098445682D+05	1.038650130D+02	2.309332330D+00	1.330517507D-04	-4.426433390D-08				
6.711419150D-12	-3.374128000D-16		3.636642690D+04	2.168088517D+01				

Ta Hf:Gurvich,1982 p85. Moore,1971. Gordon,1999.

3 g 7/97 TA	1.00	0.00	0.00	0.00	0.00	0	180.9479000	782518.638
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.150907339D+04	4.780730430D+01	3.185588390D+00	-5.366528160D-03	1.288379705D-05				
-1.045798666D-08	3.050617695D-12		9.299797630D+04	5.336056610D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.689726898D+06	-5.986854660D+03	9.565039670D+00	-2.511649459D-03	6.443031170D-07				
-7.189237250D-11	3.113352070D-15		1.306710983D+05	-4.335096270D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-8.413419560D+08	6.381509040D+05	-1.856031850D+02	2.797353600D-02	-2.073321805D-06				
7.397299170D-11	-1.017863944D-15		-4.836410620D+06	1.607007750D+03				

Ta+ Moore,1971. Gordon,1999.

3 g 7/97 TA	1.00E	-1.00	0.00	0.00	0.00	0	180.9473514	1549679.335
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.869712865D+05	-3.084920994D+03	1.430679704D+01	-1.984772164D-02	1.951445133D-05				
-8.970946030D-09	1.501974665D-12		2.013828712D+05	-6.306427830D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.656142130D+06	-1.254073524D+04	1.865022579D+01	-7.943274660D-03	2.151786937D-06				
-2.816764844D-10	1.413722944D-14		2.636876455D+05	-1.065864286D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.724273560D+07	-3.405709310D+04	1.630056321D+01	-2.064987830D-03	1.616826024D-07				
-5.752060330D-12	7.636581870D-17		4.405115500D+05	-1.040237652D+02				

Ta- Hotop,1985. Gordon,1999.

3 g 9/97 TA	1.00E	1.00	0.00	0.00	0.00	0	180.9484486	745469.429
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.873982301D+05	-1.681268679D+03	6.480040150D+00	-2.254355782D-04	2.028434876D-06				
-4.679801430D-09	1.997027996D-12		9.793496020D+04	-2.049618155D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.235467480D+06	1.101056361D+04	-4.736911070D+00	2.503562129D-03	-4.821851690D-07				
4.886408030D-11	-2.030547835D-15		1.574699408D+04	6.491802700D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.149884030D+05	1.227972146D+03	2.209211582D+00	3.401090760D-05	-2.136872502D-09				
6.906775410D-14	-9.017779200D-19		8.249065600D+04	1.195636187D+01				

## Appendix D (continued)

TaCL5 Chase,1998 p923.

2 j12/74 TA	1.00CL	5.00	0.00	0.00	0.00	0.00	0 358.2129000	-764835.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	26869.100
6.306483290D+04	-1.771221442D+03	2.255083356D+01	-1.360238041D-02	1.613009806D-05				
-1.016307761D-08	2.631917453D-12						-8.792737110D+04	-8.097864282D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	26869.100
-1.426444545D+05	-3.894340320D+01	1.603142370D+01	-1.333676355D-05	3.084307611D-09				
-3.663930060D-13	1.745841795D-17						-9.701297170D+04	-4.256986372D+01

TaO Gurvich,1982 pt1 p86 pt2 p89.

3 tpis89 TA	1.000	1.00	0.00	0.00	0.00	0 196.9473000	242534.705	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	8766.105
-1.395738049D+04	3.945236990D+02	-6.301696410D-02	1.308595441D-02	-1.862339730D-05				
1.366155583D-08	-3.924551230D-12						2.645195419D+04	2.741671469D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	8766.105
6.106591120D+06	-1.984135246D+04	2.815797433D+01	-1.330045882D-02	3.876807490D-06				
-5.068872770D-10	2.443666035D-14						1.525814433D+05	-1.658307106D+02
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	8766.105
-1.076924766D+08	1.287348862D+04	1.361132509D+01	-1.443306356D-03	9.697469230D-08				
-3.170023830D-12	4.113579900D-17						-1.302536682D+05	-6.687940680D+01

TaO2 Gurvich,1982 pt1 p89 pt2 p91.

2 tpis82 TA	1.000	2.00	0.00	0.00	0.00	0 212.9467000	-173662.006	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	10699.099
1.516356303D+04	7.058414760D+01	6.918516990D-01	2.020605733D-02	-2.928317413D-05				
2.081417374D-08	-5.751106690D-12						-2.212199468D+04	2.484662500D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	10699.099
1.297565964D+06	-4.149217430D+03	1.041680373D+01	-1.045478838D-03	2.754904271D-07				
-3.297043130D-11	1.356249074D-15						3.418985670D+03	-3.392642790D+01

Ti Hf:Cox,1989. Sugar,1985. Gordon,1999.

3 g 7/97 TI	1.00	0.00	0.00	0.00	0.00	0 47.8670000	473000.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7539.141
-4.570179400D+04	6.608092020D+02	4.295257490D-01	3.615029910D-03	-3.549792810D-06				
1.759952494D-09	-3.052720871D-13						5.270947930D+04	2.026149738D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7539.141
-1.704786714D+05	1.073852803D+03	1.181955014D+00	2.245246352D-04	3.091697848D-07				
-5.740027280D-11	2.927371014D-15						4.978069910D+04	1.740431368D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7539.141
1.152797766D+09	-7.222408380D+05	1.777167465D+02	-2.008059096D-02	1.221052354D-06				
-3.811452080D-11	4.798092423D-16						5.772614540D+06	-1.518080466D+03

Ti+ Sugar,1985. Gordon,1999.

3 g 7/97 TI	1.00E	-1.00	0.00	0.00	0.00	0 47.8664514	1137624.029	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7899.829
1.707457044D+05	-1.727524602D+03	9.615885330D+00	-1.089655060D-02	8.201809650D-06				
-2.871464413D-09	3.420382976D-13						1.447897558D+05	-3.463143660D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7899.829
-7.685463080D+05	2.545868100D+03	3.423862780D-01	7.099901360D-04	2.706231875D-08				
-2.371660100D-11	1.895443077D-15						1.198821489D+05	2.484799150D+01
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7899.829
3.918035620D+07	-2.534581605D+04	9.586759720D+00	-7.584155410D-04	4.432999350D-08				
-8.442571760D-13	-4.517128089D-19						3.344440620D+05	-5.220026270D+01

Ti- Hotop,1985. Gordon,1999.

3 g 9/97 TI	1.00E	1.00	0.00	0.00	0.00	0 47.8675486	459203.814	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7562.614
-3.006484990D+03	2.040911689D+02	1.822638976D+00	1.245254812D-03	-1.309239865D-06				
7.372143220D-10	-1.724319779D-13						5.346772050D+04	1.205926588D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7562.614
2.341117640D+04	2.580413872D+00	2.497754577D+00	9.769072040D-07	-2.280024955D-10				
2.717202291D-14	-1.295670294D-18						5.454662180D+04	7.999823950D+00
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	7562.614
1.417514172D+04	5.638799640D+00	2.498751709D+00	1.426579908D-07	-8.889194940D-12				
2.867172222D-16	-3.746329300D-21						5.451843520D+04	7.994109450D+00

TiCL Chase,1998 p808.

2 j12/68 TI	1.00CL	1.00	0.00	0.00	0.00	0 83.3200000	150850.926	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	9680.626
-1.714177839D+04	3.103259047D+02	8.920935980D-01	1.383436793D-02	-1.885370354D-05				
1.212085912D-08	-3.032162427D-12						1.558066453D+04	2.244778384D+01
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0 4.0 0.0	9680.626
-9.633225420D+05	2.868829781D+03	1.973820676D+00	-1.752668011D-03	-4.255434360D-07				
5.049103400D-11	-2.304720715D-15						-1.811011561D+03	2.319450287D+01

## Appendix D (continued)

TiCL2 Chase,1998 p866.  
 2 j12/68 TI 1.00CL 2.00 0.00 0.00 0.00 0 118.7730000 -237230.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13545.270  
 1.324354656D+04-5.762829320D+02 9.640047290D+00-4.475120950D-03 5.398794870D-06  
 -3.525800490D-09 9.746004550D-13 -2.792066683D+04-2.218347625D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13545.270  
 -3.190012950D+06 1.015763826D+04-4.840794770D+00 6.822006340D-03-1.700753270D-06  
 2.118106588D-10-1.041245457D-14 -9.480982980D+04 7.823195948D+01

TiCL3 Chase,1998 p887.  
 2 j12/68 TI 1.00CL 3.00 0.00 0.00 0.00 0 154.2260000 -539320.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15374.947  
 1.243282268D+05-2.320728253D+03 1.779895274D+01-1.160889348D-02 1.006643154D-05  
 -4.811940690D-09 1.006186828D-12 -5.609602510D+04-6.732754065D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15374.947  
 -9.408792310D+04-1.255351109D+02 1.066923972D+01-2.637456897D-04 7.959169350D-08  
 -1.176740054D-11 6.416223480D-16 -6.769114680D+04-2.369164216D+01

TiCL4 Chase,1998 p906.  
 2 j12/67 TI 1.00CL 4.00 0.00 0.00 0.00 0 189.6790000 -763160.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21613.541  
 8.187196800D+04-1.758323850D+03 1.892512121D+01-1.133495876D-02 1.251952037D-05  
 -7.422681330D-09 1.825440187D-12 -8.672923110D+04-6.769594291D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21613.541  
 -1.432562278D+05-4.316774850D+01 1.303337752D+01-1.371365738D-05 3.093403483D-09  
 -3.604245160D-13 1.691384523D-17 -9.588947000D+04-3.247541011D+01

TiO Gurvich,1982 pt1 p99 pt2 p101.  
 3 tpis89 TI 1.000 1.00 0.00 0.00 0.00 0 63.8664000 49503.615  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9593.115  
 -1.168152460D+04 4.542565650D+02-1.139144613D-01 1.275432333D-02-1.727656935D-05  
 1.187369403D-08-3.236579370D-12 2.924306353D+03 2.702903947D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9593.115  
 2.330644030D+06-7.415793860D+03 1.281799311D+01-4.344555950D-03 1.186303111D-06  
 -1.367644275D-10 5.703212250D-15 5.144841360D+04-5.793994240D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9593.115  
 1.660288147D+08-1.051853502D+05 2.749141313D+01-1.681501753D-03 4.884078370D-08  
 -4.721389750D-13-2.405919722D-18 8.399156070D+05-2.030813444D+02

TiO+ Gurvich,1982 pt1 p104 pt2 p103.  
 3 tpis82 TI 1.000 1.00E -1.00 0.00 0.00 0 63.8658514 685321.011  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9213.111  
 3.691256250D+04-1.492825538D+02 2.624977257D+00 5.818627130D-03-7.529662110D-06  
 4.744154350D-09-1.186916989D-12 8.241551170D+04 1.095428726D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9213.111  
 3.421329530D+05-2.161851060D+03 8.025175660D+00-2.708700692D-03 1.004583805D-06  
 -1.505766850D-10 8.045658110D-15 9.362646990D+04-2.261587887D+01  
 6000.000 20000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9213.111  
 6.877707550D+07-4.060032000D+04 1.371193858D+01-6.905832140D-04 2.394468882D-08  
 -4.056406410D-13 2.475735466D-18 4.034409840D+05-8.020740780D+01

TiOCL Chase,1998 p796.  
 2 j 9/63 TI 1.000 1.00CL 1.00 0.00 0.00 0 99.3194000 -244262.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12142.701  
 3.545856510D+04-6.295287140D+02 7.370176300D+00 3.302019140D-03-6.121458750D-06  
 4.735880250D-09-1.374690357D-12 -2.797087903D+04-1.294470159D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12142.701  
 -1.273059873D+05-1.11118850D+02 7.582888080D+00-3.312871800D-05 7.314014090D-09  
 -8.378822260D-13 3.879275060D-17 -3.139356857D+04-1.247104274D+01

TiOCL2 Chase,1998 p843.  
 2 j 9/63 TI 1.000 1.00CL 2.00 0.00 0.00 0 134.7724000 -545552.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16710.010  
 3.289052460D+04-7.389188590D+02 1.055976857D+01 1.577742341D-03-3.907182100D-06  
 3.290576530D-09-9.949471750D-13 -6.448410700D+04-2.417469934D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16710.010  
 -1.322951633D+05-9.691212050D+01 1.007240769D+01-2.897248531D-05 6.401775040D-09  
 -7.338452600D-13 3.399282670D-17 -6.847409640D+04-1.975043469D+01

TiO2 Chase,1998 p1762 12/73. Jacox,1998.  
 2 g10/99 TI 1.000 2.00 0.00 0.00 0.00 0 79.8658000 -305430.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11351.690  
 -1.710545601D+03 2.721435528D+02 5.961378960D-01 1.925463599D-02-2.665500165D-05  
 1.811109197D-08-4.876710470D-12 -3.912241770D+04 2.408605889D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11351.690  
 1.546299764D+05-1.046256880D+03 7.788985830D+00-1.546805714D-04-7.059935950D-08  
 3.100244802D-11-2.494725430D-15 -3.266336750D+04-1.591534660D+01



## Appendix D (continued)

U                      Gurvich,1982 pt1 p184 pt2 p201. Blaise,1976.

3 g 7/00 U	1.00	0.00	0.00	0.00	0.00	0	238.0289100	535000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.965737750D+04	-1.070351517D+03	8.075842310D+00	-1.060034069D-02	9.256548010D-06				
-3.219899760D-09	4.058048809D-13		6.866513700D+04	-2.240521678D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.092498960D+06	1.274888349D+04	-1.218707506D+01	7.258105680D-03	-7.787775070D-07				
-3.844353850D-11	7.066508567D-15		-1.699372664D+04	1.155026301D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.424676814D+08	1.022495503D+05	-2.321762289D+00	-7.433177460D-04	9.674993970D-08				
-4.159452280D-12	6.313829223D-17		-8.137559280D+05	7.333489176D+01				

UF                      Gurvich,1982 pt1 p202 pt2 p224.

3 tpis82 U	1.00F	1.00	0.00	0.00	0.00	0	257.0273132	-49250.737
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.725533463D+04	-1.698985561D+03	5.902926430D+00	1.841977309D-02	-4.633174310D-05				
4.376657200D-08	-1.451876566D-11		2.086455917D+03	-1.186592944D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.325439370D+06	1.533967086D+04	-1.175044398D+01	9.647210930D-03	-2.498778190D-06				
3.155572896D-10	-1.544694839D-14		-1.057196525D+05	1.220828149D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.021978468D+08	-1.196840152D+05	3.263355240D+01	-2.553105588D-03	1.191730174D-07				
-2.677714445D-12	2.360089903D-17		9.473656850D+05	-2.396788565D+02				

UF+                      Gurvich,1982 pt1 p203 pt2 p226.

3 tpis82 U	1.00F	1.00E	-1.00	0.00	0.00	0	257.0267646	557058.967
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.622640597D+06	-1.917326611D+04	8.759461220D+01	-1.699915707D-01	1.861251683D-04				
-1.036176702D-07	2.324287412D-11		1.616709643D+05	-4.806891249D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.395091840D+05	-2.923962095D+03	1.008511948D+01	-2.425945123D-03	5.928725480D-07				
-6.795845540D-11	3.152666445D-15		8.267291220D+04	-3.307089704D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.357726300D+07	-1.105107069D+04	1.891324705D+00	1.246403421D-03	-1.128508026D-07				
4.314527550D-12	-6.027569830D-17		1.776673362D+05	2.409952635D+01				

UF-                      Gurvich,1982 pt1 p204 pt2 p228.

3 g12/99 U	1.00F	1.00E	1.00	0.00	0.00	0	257.0278618	-155679.193
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.692327860D+03	-1.491979606D+02	4.033988520D+00	2.857429445D-03	-5.171702560D-06				
3.985379110D-09	-9.470355440D-13		-1.915281695D+04	6.059243838D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.311143560D+06	1.974817938D+04	-2.760304763D+01	2.276806261D-02	-6.888741720D-06				
9.483511060D-10	-4.910688100D-14		-1.380801290D+05	2.240758537D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.090384299D+08	1.824173856D+05	-3.570033800D+01	4.596835280D-03	-2.809511961D-07				
9.028550240D-12	-1.169274383D-16		-1.475954920D+06	3.592431751D+02				

UF2                      Gurvich,1982 pt1 p205 pt2 p230.

3 tpis82 U	1.00F	2.00	0.00	0.00	0.00	0	276.0257164	-535036.715
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.882492020D+04	4.454930860D+02	4.718009190D+00	1.648911480D-03	8.696243010D-06				
-1.207439921D-08	4.536793910D-12		-6.855329330D+04	1.159725423D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.716776820D+05	3.224236860D+02	8.214090630D+00	-1.407413780D-04	6.541178050D-09				
1.818915497D-12	-2.287963719D-16		-6.995235050D+04	-9.648963156D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.833722170D+06	-5.166288400D+03	1.000042588D+01	-3.502166850D-04	1.973413760D-08				
-5.613962470D-13	6.472362570D-18		-2.897767010D+04	-2.492966720D+01				

UF2+                      Gurvich,1982 pt1 p207 pt2 p232.

3 tpis82 U	1.00F	2.00E	-1.00	0.00	0.00	0	276.0251678	70445.527
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
5.439010160D+03	-1.507096256D+02	6.873485190D+00	1.530973969D-03	-3.316694310D-06				
2.949453335D-09	-8.281706540D-13		7.256014910D+03	-2.205491833D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.779149610D+06	1.298737504D+04	-1.027930641D+01	1.048838051D-02	-2.651047812D-06				
3.116973593D-10	-1.417216291D-14		-7.433440200D+04	1.189131079D+02				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.003702250D+07	4.886273610D+04	-2.192209667D-01	6.378651730D-04	-3.372669300D-08				
9.777729090D-13	-1.189890068D-17		-3.936562000D+05	6.595164355D+01				

## Appendix D (continued)

UF2- Gurvich,1982 pt1 p208 pt2 p234.

3	tpis82 U	1.00F	2.00E	1.00	0.00	0.00	0	276.0262650	-678233.195
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.060491730D+05	-9.404254660D+03	4.448392770D+01	-6.868558770D-02	6.777809920D-05					
-3.338827680D-08	6.604851620D-12		-3.603306130D+04	-2.261594249D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.038231855D+07	-2.840113518D+04	3.498533370D+01	-1.053216396D-02	1.924620470D-06					
-1.698749570D-10	5.709858890D-15		1.001572794D+05	-2.094039075D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.046229980D+07	3.524957180D+04	-8.601752150D-01	8.947422820D-04	-5.540675440D-08					
1.776021844D-12	-2.307535574D-17		-3.584621110D+05	6.877566575D+01					

UF3 Gurvich,1982 pt1 p210 pt2 p237.

3	tpis82 U	1.00F	3.00	0.00	0.00	0.00	0	295.0241196	-1060958.597
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.071027207D+04	-6.340789470D+02	1.114030799D+01	-2.937554125D-04	-1.865390371D-06					
2.371819470D-09	-7.446754070D-13		-1.271838141D+05	-2.348962529D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.828876420D+06	1.296891783D+04	-7.265554290D+00	1.048289752D-02	-2.649840687D-06					
3.115594509D-10	-1.416579400D-14		-2.113615913D+05	1.054464687D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-9.007768940D+07	4.885212250D+04	2.783068500D+00	6.376088800D-04	-3.371098360D-08					
9.772726250D-13	-1.189242739D-17		-5.307242640D+05	5.256841035D+01					

UF3+ Gurvich,1982 pt1 p211 pt2 p239.

3	tpis82 U	1.00F	3.00E	-1.00	0.00	0.00	0	295.0235710	-284745.430
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.984155890D+05	3.480892440D+03	-2.519603507D+00	2.283749282D-02	-2.168844780D-05					
1.111265790D-08	-2.350882012D-12		-5.550889200D+04	5.853815975D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.196316388D+06	3.972785070D+03	4.535907110D+00	4.133416150D-03	-1.097960689D-06					
1.319641252D-10	-6.101129180D-15		-6.199541740D+04	2.137623045D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.490516590D+07	2.285903928D+04	7.869516510D+00	1.274792626D-04	-5.228047920D-09					
1.360286305D-13	-1.645113815D-18		-2.269266296D+05	6.797911871D+00					

UF3- Gurvich,1982 pt1 p212 pt2 p241.

3	tpis82 U	1.00F	3.00E	1.00	0.00	0.00	0	295.0246682	-1186440.771
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.315187300D+05	2.534197822D+03	-3.180714590D+00	2.932741422D-02	-2.856912260D-05					
1.345804152D-08	-2.465442912D-12		-1.580387746D+05	5.973605435D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.910053149D+05	-5.069181310D+02	1.181482258D+01	-1.711879404D-04	-9.384839180D-08					
2.242009537D-11	-1.428195280D-15		-1.438628681D+05	-2.774680411D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.944714123D+07	1.429185303D+04	7.239366640D+00	2.897026663D-04	-1.704156160D-08					
5.276150470D-13	-6.688352280D-18		-2.573053031D+05	1.122428161D+01					

UF4 Gurvich,1982 pt1 p215 pt2 p244.

3	tpis82 U	1.00F	4.00	0.00	0.00	0.00	0	314.0225228	-1606157.418
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.007852380D+04	-9.693493550D+02	2.069596355D+01	-2.564852637D-02	4.195860120D-05					
-3.201013390D-08	9.422076860D-12		-1.931626334D+05	-7.172362935D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.230291173D+06	3.876463790D+03	7.621625910D+00	4.094525220D-03	-1.088530094D-06					
1.308042117D-10	-6.044390870D-15		-2.214142920D+05	6.270300658D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.422199930D+07	2.244095755D+04	1.096208609D+01	1.168958941D-04	-4.568843620D-09					
1.147904592D-13	-1.368068374D-18		-3.836270440D+05	-8.486934342D+00					

UF4+ Gurvich,1982 pt1 p216 pt2 p246.

3	tpis82 U	1.00F	4.00E	-1.00	0.00	0.00	0	314.0219742	-641539.484
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.848956330D+04	-1.343282151D+03	1.646334809D+01	-7.196079860D-03	1.147165041D-05					
-8.705877980D-09	2.501076195D-12		-7.405048200D+04	-5.295285535D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.617630159D+06	3.765934770D+03	9.166138530D+00	2.426641067D-03	-5.695320300D-07					
6.021096600D-11	-2.438874329D-15		-1.061910645D+05	-4.162641042D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.790280948D+07	1.464555692D+04	1.168522991D+01	5.249951330D-05	-1.762380856D-10					
-5.000071600D-14	1.088450028D-18		-2.028630553D+05	-1.708462849D+01					

## Appendix D (continued)

UF4- Gurvich,1982 pt1 p217 pt2 p248.

3 tps	82 U	1.00F	4.00E	1.00	0.00	0.00	0	314.0230714	-1728334.866
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.203179690D+04	-1.374343862D+03	1.640877729D+01	-4.363066270D-03	2.460407959D-06					
-1.498144731D-10	-1.239417075D-13								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.639200110D+06	1.626824426D+04	-9.595291050D+00	1.441556535D-02	-4.008173850D-06					
5.140230790D-10	-2.511687821D-14								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.308421305D+08	8.061319300D+04	-3.939161520D+00	1.853747295D-03	-1.116700599D-07					
3.508474880D-12	-4.490622440D-17								

UF5 Gurvich,1982 pt1 p219 pt2 p251.

3 tps	82 U	1.00F	5.00	0.00	0.00	0.00	0	333.0209260	-1949823.884
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.615769193D+05	-2.976611537D+03	2.537542420D+01	-1.930105670D-02	2.561852107D-05					
-1.747402896D-08	4.732059380D-12								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.695373880D+06	3.735425350D+03	1.218748040D+01	2.418608203D-03	-5.678526160D-07					
6.002765610D-11	-2.430740809D-15								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.820007103D+07	1.475725044D+04	1.466020135D+01	5.538728810D-05	-3.572588510D-10					
-4.414506670D-14	1.011890437D-18								

UF5+ Gurvich,1982 pt1 p220 pt2 p253.

3 tps	82 U	1.00F	5.00E	-1.00	0.00	0.00	0	333.0203774	-853617.242
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.626519713D+05	-2.915370389D+03	2.436168077D+01	-1.382199656D-02	1.339849041D-05					
-7.078572690D-09	1.573404040D-12								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.628478263D+05	-1.174047323D+02	1.608988291D+01	-3.665516710D-05	8.221494970D-09					
-9.537160520D-13	4.460145080D-17								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.772763820D+04	-1.534892435D+02	1.603372733D+01	-3.833472040D-06	2.377658266D-10					
-7.638474870D-15	9.946126940D-20								

UF5- Gurvich,1982 pt1 p221 pt2 p255.

3 tps	82 U	1.00F	5.00E	1.00	0.00	0.00	0	333.0214746	-2289431.237
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.142130934D+05	2.020611008D+03	7.508491820D+00	1.640034396D-02	-1.562795472D-05					
7.990246010D-09	-1.671674534D-12								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.331518187D+06	3.905516860D+03	1.058727667D+01	4.112507270D-03	-1.093277930D-06					
1.314215436D-10	-6.075778270D-15								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.492648300D+07	2.277621599D+04	1.388769935D+01	1.254140874D-04	-5.100027930D-09					
1.319174409D-13	-1.591595740D-18								

UF6 Gurvich,1982 pt1 p223 pt2 p257.

3 tps	82 U	1.00F	6.00	0.00	0.00	0.00	0	352.0193292	-2148641.648
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.915674060D+05	-3.426391610D+03	2.800395890D+01	-1.326392086D-02	1.107123764D-05					
-4.821754110D-09	8.325132450D-13								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.409027920D+05	-1.458950046D+02	1.910902533D+01	-4.358451130D-05	9.617604660D-09					
-1.100915551D-12	5.092645080D-17								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.639780713D+05	-8.680089820D+01	1.901877513D+01	-2.107561344D-06	1.295346553D-10					
-4.136090060D-15	5.365237680D-20								

UF6- Gurvich,1982 pt1 p224 pt2 p258.

3 tps	82 U	1.00F	6.00E	1.00	0.00	0.00	0	352.0198778	-2691306.150
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.569230858D+05	-3.027279940D+03	2.701442427D+01	-1.136860992D-02	8.298576160D-06					
-2.582889593D-09	2.790817248D-13								
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.699676848D+06	-6.574459670D+03	2.241731997D+01	6.057799710D-04	-4.517491710D-07					
7.821820470D-11	-4.560334720D-15								
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.865804610D+07	4.174825500D+04	1.201141201D+01	6.958372750D-04	-4.049760430D-08					
1.262006447D-12	-1.620083625D-17								

## Appendix D (continued)

UO Gurvich,1982 pt1 p186 pt2 p205.

3 tps82 U	1.000	1.00	0.00	0.00	0.00	0	254.0283100	30488.589
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.007249615D+06	-1.287190666D+04	5.993123920D+01	-1.003445164D-01	8.529345550D-05				
-2.634105066D-08	-5.350649790D-13		6.627442520D+04	-3.226786779D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.458660003D+06	3.942652160D+03	5.016030720D+00	-5.450639470D-04	2.096321351D-07				
-2.654652526D-11	1.361108472D-15		-2.665149645D+04	5.580598689D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.643829702D+08	-6.893889290D+04	1.274655043D+01	3.898071910D-04	-8.455141670D-08				
4.053706450D-12	-6.354764880D-17		5.854610850D+05	-7.355640184D+01				

UO+ Gurvich,1982 pt1 p189 pt2 p207.

3 tps82 U	1.000	1.00E	-1.00	0.00	0.00	0	254.0277614	580971.927
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.562834007D+04	-1.224921454D+02	3.324146160D+00	2.467496097D-03	-6.851856740D-07				
5.552073190D-11	-5.893012030D-14		6.952999740D+04	9.583869879D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.063714748D+05	-1.793716133D+03	8.024449050D+00	-1.565116442D-03	5.066033910D-07				
-7.373977470D-11	4.074766430D-15		7.789085840D+04	-2.115284250D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.623486280D+07	4.390299020D+04	-9.206507600D+00	2.335209239D-03	-1.678226513D-07				
5.653921370D-12	-7.297202790D-17		-2.648708363D+05	1.200887991D+02				

UOF Gurvich,1982 pt1 p225 pt2 p259.

2 tps82 U	1.000	1.00F	1.00	0.00	0.00	0	273.0267132	-542182.744
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.861248470D+02	5.162286900D+01	4.888962520D+00	7.265633560D-03	-1.134176875D-05				
8.509041750D-09	-2.354655485D-12		-6.719813380D+04	8.269521875D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.805936010D+06	1.295207909D+04	-1.025373631D+01	1.047841671D-02	-2.648894949D-06				
3.114551623D-10	-1.416111895D-14		-1.478976701D+05	1.184570601D+02				

UOF2 Gurvich,1982 pt1 p226 pt2 p261.

2 tps82 U	1.000	1.00F	2.00	0.00	0.00	0	292.0251164	-1115510.264
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.106618310D+04	-1.014150169D+02	1.371057013D+01	-1.659931694D-02	3.082352584D-05				
-2.490530206D-08	7.580617640D-12		-1.374686016D+05	-3.470029665D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.198944060D+06	3.852173410D+03	4.639109750D+00	4.087738440D-03	-1.087067018D-06				
1.306398384D-10	-6.036901520D-15		-1.612637583D+05	2.018237189D+01				

UOF3 Gurvich,1982 pt1 p229 pt2 p264.

2 tps82 U	1.000	1.00F	3.00	0.00	0.00	0	311.0235196	-1510638.039
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.249256374D+05	-2.111719498D+03	1.844931536D+01	-1.041493583D-02	1.469002962D-05				
-1.049770051D-08	2.922353602D-12		-1.743844024D+05	-6.649285435D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.658296049D+06	3.714434680D+03	9.202425540D+00	2.412862293D-03	-5.666241720D-07				
5.989062110D-11	-2.424534810D-15		-2.105491714D+05	-5.670532802D+00				

UOF4 Gurvich,1982 pt1 p230 pt2 p265.

2 tps82 U	1.000	1.00F	4.00	0.00	0.00	0	330.0219228	-1785611.531
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.437164405D+05	-2.496730363D+03	2.104827038D+01	-4.692561330D-03	8.741718650D-07				
1.517555623D-09	-7.768799740D-13		-2.061284178D+05	-8.246219615D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.996190288D+05	-1.677276501D+02	1.612494871D+01	-4.984414460D-05	1.098253497D-08				
-1.255803231D-12	5.804480980D-17		-2.195459260D+05	-5.024484645D+01				

UO2 Gurvich,1982 pt1 p193 pt2 p211.

3 tps82 U	1.000	2.00	0.00	0.00	0.00	0	270.0277100	-477819.903
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.129650727D+05	4.270730270D+02	8.413694010D+00	-9.764280000D-03	2.199903691D-05				
-1.907665954D-08	6.029889910D-12		-6.251443300D+04	-1.300704863D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.190542635D+06	3.832186350D+03	2.153236312D+00	4.082351910D-03	-1.085924847D-06				
1.305134065D-10	-6.031215750D-15		-8.367618010D+04	2.590742388D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.415894110D+07	2.241359238D+04	5.468051300D+00	1.162219348D-04	-4.527223330D-09				
1.134573678D-13	-1.350744532D-18		-2.459740375D+05	1.133700240D+01				

## Appendix D (continued)

UO2+ Gurvich,1982 pt1 p194 pt2 p213.

3 tps82 U	1.000	2.00E	-1.00	0.00	0.00	0	270.0271614	51493.919
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.488023380D+04	-6.489236420D+02	6.874243560D+00	2.281949316D-03	1.859218752D-07				
-1.849509036D-09	8.149965330D-13		7.891740230D+03	-1.028257233D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.589957420D+06	3.657746070D+03	3.746785420D+00	2.394401448D-03	-5.624101440D-07				
5.939451640D-11	-2.401047056D-15		-2.048558817D+04	1.464015614D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.778324150D+07	1.456161876D+04	6.203516610D+00	5.043474040D-05	-4.877674180D-11				
-5.408292310D-14	1.141506994D-18		-1.172230791D+05	2.164589095D+00				

UO2- Gurvich,1982 pt1 p195 pt2 p215.

3 tps82 U	1.000	2.00E	1.00	0.00	0.00	0	270.0282586	-573700.021
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.341971310D+04	-7.196118500D+02	8.308241620D+00	9.626455450D-04	-3.583733980D-06				
3.473554580D-09	-1.022793120D-12		-6.718169870D+04	-1.606030120D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.738251640D+05	3.228534420D+03	-2.805114576D-01	6.607310710D-03	-2.070291015D-06				
2.851708013D-10	-1.466578192D-14		-8.893436180D+04	4.145760316D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.053612192D+08	6.331803380D+04	-5.853591580D+00	1.472289928D-03	-8.933245500D-08				
2.824078529D-12	-3.633249210D-17		-5.772299570D+05	1.092379584D+02				

UO2F Gurvich,1982 pt1 p226 pt2 p260.

2 tps82 U	1.000	2.00F	1.00	0.00	0.00	0	289.0261132	-997934.842
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.321792390D+04	-1.327082127D+03	1.240125390D+01	-4.084151010D-03	7.331593480D-06				
-5.987404880D-09	1.787869209D-12		-1.157526888D+05	-3.415298625D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.614277202D+06	3.712771860D+03	6.203308820D+00	2.412618055D-03	-5.665888020D-07				
5.988823520D-11	-2.424485602D-15		-1.478357384D+05	8.736139132D+00				

UO2F2 Gurvich,1982 pt1 p228 pt2 p263.

2 tps82 U	1.000	2.00F	2.00	0.00	0.00	0	308.0245164	-1354232.027
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
9.959874300D+04	-1.530010701D+03	1.358992177D+01	5.370655800D-03	-1.141444341D-05				
9.301197040D-09	-2.781220538D-12		-1.580310734D+05	-4.196260275D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.636552036D+05	-2.032835065D+02	1.315092994D+01	-6.006486830D-05	1.321137913D-08				
-1.508668985D-12	6.966182750D-17		-1.664444818D+05	-3.566258175D+01				

UO3 Gurvich,1982 pt1 p197 pt2 p218.

3 tps82 U	1.000	3.00	0.00	0.00	0.00	0	286.0271100	-799239.411
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
6.637677040D+04	-7.582646580D+02	7.112844710D+00	1.322149697D-02	-2.106191042D-05				
1.545856318D-08	-4.378566290D-12		-9.413369350D+04	-8.588030428D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.097362721D+06	2.808784061D+03	5.966121470D+00	2.861871152D-03	-1.052843810D-06				
1.849985929D-10	-1.102849619D-14		-1.173360017D+05	6.672828312D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.632929098D+09	-9.419553920D+05	2.142384145D+02	-2.094922993D-02	1.131511326D-06				
-3.129107183D-11	3.504914590D-16		7.448065370D+06	-1.824526663D+03				

UO3- Gurvich,1982 pt1 p198 pt2 p220.

3 tps82 U	1.000	3.00E	1.00	0.00	0.00	0	286.0276586	-1305154.518
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.000143902D+05	-1.448443754D+03	1.217532415D+01	-2.944956748D-03	5.675228000D-06				
-4.916710420D-09	1.525185713D-12		-1.519253376D+05	-3.471731375D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.632938634D+06	3.667495410D+03	6.240030650D+00	2.396952522D-03	-5.629490230D-07				
5.945413130D-11	-2.403730982D-15		-1.845927385D+05	7.032059012D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.781940595D+07	1.456116475D+04	8.703650860D+00	5.041649230D-05	-4.751131470D-11				
-5.412647410D-14	1.142098108D-18		-2.812591514D+05	-5.495926098D+00				

V Hf:Gurvich,1982 p59. Sugar,1985. Gordon,1999.

3 g 7/97 V	1.00	0.00	0.00	0.00	0.00	0	50.9415000	517267.064
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.535376020D+04	5.593338510D+02	2.675543482D+00	-6.243049630D-03	1.565902337D-05				
-1.372845314D-08	4.168388810D-12		5.820664360D+04	9.524567490D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.200390300D+06	-5.027005300D+03	1.058830594D+01	-5.044326100D-03	1.488547375D-06				
-1.785922508D-10	8.113013866D-15		9.170740910D+04	-4.768336320D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.456040166D+09	-1.339992028D+06	2.781039851D+02	-2.638937359D-02	1.303527149D-06				
-3.214680330D-11	3.099999094D-16		1.087152043D+07	-2.439954380D+03				

## Appendix D (continued)

V+ Sugar,1985. Gordon,1999.

3 g 7/97 V	1.00E	-1.00	0.00	0.00	0.00	0	50.9409514	1173745.411
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.568834460D+04	-8.415273820D+02	7.559232710D+00	-1.441722656D-02	2.038356397D-05				
-1.289073883D-08	3.065656561D-12		1.444478191D+05	-1.991067645D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.347072054D+06	-9.021197190D+03	1.477349798D+01	-6.891896880D-03	1.968884877D-06				
-2.539798544D-10	1.226783122D-14		1.958351444D+05	-7.855592930D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.516527258D+08	-1.866476656D+05	5.633587110D+01	-7.198536950D-03	5.074401490D-07				
-1.699749225D-11	2.157800037D-16		1.585980536D+06	-4.512822600D+02				

V- Hotop,1985. Gordon,1999.

3 g 9/97 V	1.00E	1.00	0.00	0.00	0.00	0	50.9420486	460386.063
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.799273560D+03	2.313840448D+02	1.725608190D+00	1.429275357D-03	-1.506038188D-06				
8.491815170D-10	-1.987980413D-13		5.347402920D+04	1.261900982D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.600100430D+04	2.096334097D+00	2.498006548D+00	8.991278840D-07	-2.139749508D-10				
2.581021334D-14	-1.240812796D-18		5.470007080D+04	7.977900240D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.601102910D+04	5.820974900D+00	2.498705489D+00	1.484212570D-07	-9.272956840D-12				
2.997799727D-16	-3.924862230D-21		5.466692550D+04	7.974557420D+00				

VCL4 Nagarajan,1963. Creighton,1966. Blankenship,1962.

2 g10/00 V	1.00CL	4.00	0.00	0.00	0.00	0	192.7535000	-527058.480
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.719834710D+04	-1.702854040D+03	1.882697965D+01	-1.130896832D-02	1.266950765D-05				
-7.625019340D-09	1.907582465D-12		-5.863748540D+04	-6.559171106D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.717776251D+06	4.550441050D+03	8.164464800D+00	2.224875998D-03	-4.094111780D-07				
3.271787500D-11	-8.858690800D-16		-9.690620060D+04	4.348293098D+00				

VN Chase,1998 p1616.

2 j12/73 V	1.00N	1.00	0.00	0.00	0.00	0	64.9482000	523000.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.581737285D+04	4.868165420D+02	-1.045200388D+00	1.685261043D-02	-2.334616543D-05				
1.588710050D-08	-4.279080880D-12		5.981481400D+04	3.144995263D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.018619667D+06	-3.932305570D+03	9.856823610D+00	-3.289221710D-03	1.005181767D-06				
-1.243211436D-10	5.486776560D-15		8.557318340D+04	-3.552830762D+01				

VO Gurvich,1982 pt1 p62 pt2 p64.

3 tpis89 V	1.000	1.00	0.00	0.00	0.00	0	66.9409000	148582.706
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.311619784D+04	3.747816970D+02	9.300834860D-02	1.244977714D-02	-1.688540028D-05				
1.142443381D-08	-3.040589320D-12		1.523789920D+04	2.536811755D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.986190283D+06	-1.011344974D+04	1.718161749D+01	-7.876705030D-03	2.562279547D-06				
-3.547400350D-10	1.770268056D-14		7.961254880D+04	-8.789993010D+01				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.004530292D+08	-9.008780230D+04	3.186107720D+01	-2.862639937D-03	1.440482244D-07				
-3.802861470D-12	4.195092660D-17		7.011401290D+05	-2.336810859D+02				

VO2 Gurvich,1982 pt1 p64 pt2 p66.

2 tpis82 V	1.000	2.00	0.00	0.00	0.00	0	82.9403000	-232697.655
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.678585860D+03	3.911597580D+02	-1.028549847D+00	2.401523419D-02	-3.337378810D-05				
2.283623543D-08	-6.199143100D-12		-3.074609276D+04	3.277912380D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.210632401D+05	-1.627832993D+03	9.252713100D+00	-1.572703139D-03	5.231430160D-07				
-6.476071140D-11	2.847226026D-15		-2.097306345D+04	-2.547380687D+01				

V4010 Gurvich,1982 pt1 p69 pt2 p70.

2 g10/99 V	4.000	10.00	0.00	0.00	0.00	0	363.7600000	-2825164.486
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.385739160D+05	-5.353929260D+03	2.993220131D+01	5.818836520D-02	-9.696340160D-05				
7.274756990D-08	-2.091628357D-11		-3.189349370D+05	-1.466398396D+02				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.360273270D+06	-1.341692860D+03	4.099138590D+01	-3.932265530D-04	8.628494120D-08				
-9.835944090D-12	4.535637290D-16		-3.484616120D+05	-1.907911348D+02				

## Appendix D (continued)

W Hf:Gurvich,1982 p42. Moore,1971. Moore,1970a. Gordon,1999.

3 g 4/98 W	1.00	0.00	0.00	0.00	0.00	0 183.8400000	851243.526
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6216.526
1.595223922D+05	-2.673843928D+03	2.060469727D+01	-6.252315230D-02	1.105654838D-04			
-8.453511610D-08	2.336187771D-11		1.139648616D+05	-9.011836900D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6216.526
-8.048745960D+06	1.465700424D+04	-2.508531501D-01	-2.596486992D-03	1.409225475D-06			
-2.233011706D-10	1.262640862D-14		-3.091130919D+03	3.955822190D+01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6216.526
1.421636486D+09	-4.325365550D+05	-8.841615070D+00	1.645538940D-02	-1.908373835D-06			
8.530482890D-11	-1.360501851D-15		3.994798750D+06	-1.266418236D+01			

W+ Moore,1971. Gordon,1999.

3 g 7/97 W	1.00E	-1.00	0.00	0.00	0.00	0 183.8394514	1627840.965
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6221.265
-1.969284929D+05	2.670137332D+03	-1.131686913D+01	3.308183730D-02	-3.629035500D-05			
2.066142971D-08	-4.808285562D-12		1.820950862D+05	8.552104480D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6221.265
6.387743400D+06	-2.061811463D+04	2.759291576D+01	-1.244535845D-02	3.271200490D-06			
-4.065463720D-10	1.912595872D-14		3.245174430D+05	-1.716919194D+02			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6221.265
6.839559150D+07	-8.981711810D+04	3.845720800D+01	-5.465752290D-03	4.024981150D-07			
-1.342970538D-11	1.667637540D-16		8.546932820D+05	-2.892805521D+02			

W- Hotop,1985. Gordon,1999.

3 g 1/99 W	1.00E	1.00	0.00	0.00	0.00	0 183.8405486	766391.528
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6197.428
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		9.142981370D+04	8.461169670D+00			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6197.428
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		9.142981370D+04	8.461169670D+00			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	6197.428
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00			
0.000000000D+00	0.000000000D+00		9.142981370D+04	8.461169670D+00			

WCL6 Chase,1998 p935.

2 j12/66 W	1.00CL	6.00	0.00	0.00	0.00	0 396.5580000	-493712.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	30790.955
3.339391670D+04	-1.697366080D+03	2.560612352D+01	-1.425247881D-02	1.739682668D-05			
-1.120537864D-08	2.951522890D-12		-5.673059240D+04	-9.741466299D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	30790.955
-1.516735473D+05	-3.451379250D+01	1.902867176D+01	-1.242486969D-05	2.917675103D-09			
-3.505981440D-13	1.685355887D-17		-6.535779790D+04	-5.894914959D+01			

WO Gurvich,1982 pt1 p43 pt2 p47.

3 tpis82 W	1.000	1.00	0.00	0.00	0.00	0 199.8394000	401735.711
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	9259.111
-1.933758411D+04	4.936690840D+02	-4.116148220D-01	1.307976507D-02	-1.689145619D-05			
1.092748066D-08	-2.820593541D-12		4.511017900D+04	3.002592661D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	9259.111
1.262156956D+06	-4.177263120D+03	9.358286470D+00	-2.887612220D-03	8.893933960D-07			
-8.955318700D-11	2.504359614D-15		7.313380640D+04	-3.144882290D+01			
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	9259.111
1.942009403D+08	-1.501316158D+05	4.237023540D+01	-3.309676390D-03	1.396809578D-07			
-3.039263166D-12	2.703787815D-17		1.214349290D+06	-3.296819210D+02			

WOCL4 Chase,1998 p900.

2 j 3/67 W	1.000	1.00CL	4.00	0.00	0.00	0 341.6514000	-573493.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	22271.379
2.658812693D+04	-9.336913240D+02	1.321377385D+01	1.270930811D-02	-1.964716509D-05			
1.405106974D-08	-3.899382140D-12		-6.792290790D+04	-3.594869683D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	22271.379
-3.049028285D+05	-3.539425860D+02	1.626432703D+01	-1.058245461D-04	2.340548846D-08			
-2.685852021D-12	1.245412684D-16		-7.272546740D+04	-4.991761253D+01			

WO2 Gurvich,1982 pt1 p47 pt2 p50.

2 tpis82 W	1.000	2.00	0.00	0.00	0.00	0 215.8388000	29061.744
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	10714.848
3.120918919D+03	2.413883468D+02	-3.024119184D-01	2.324333417D-02	-3.378812680D-05			
2.380934019D-08	-6.421592880D-12		1.442005265D+03	2.957655179D+01			
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0 3.0 4.0 0.0	10714.848
-7.537406680D+05	3.204643050D+03	6.701965600D-01	4.488238870D-03	-8.858328460D-07			
6.245171750D-11	-9.046613900D-16		-1.769420230D+04	3.405724010D+01			

## Appendix D (continued)

WO2CL2 Chase, 1998 p849.

2 j 3/67 W	1.000	2.00CL	2.00	0.00	0.00	0	286.7448000	-671532.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.300154480D+02	-2.438547856D+02	7.976306990D+00	1.715005722D-02	-2.487975176D-05				
1.737644163D-08	-4.771928400D-12		-8.232812400D+04	-7.844771421D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.404791730D+05	-3.068379644D+02	1.322814502D+01	-9.100220710D-05	2.006581020D-08				
-2.296837607D-12	1.062829386D-16		-8.367493060D+04	-3.491556626D+01				

WO3 Gurvich, 1982 pt1 p50 pt2 p52.

2 tpi82 W	1.000	3.00	0.00	0.00	0.00	0	231.8382000	-319725.213
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.262461460D+03	3.429391090D+01	1.573061955D+00	2.754971099D-02	-3.994827310D-05				
2.809371537D-08	-7.777545730D-12		-4.001733270D+04	1.857409963D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.732203640D+06	-6.284719780D+03	1.681358864D+01	-3.472089360D-03	8.079935800D-07				
-6.589378720D-11	1.142928957D-15		-2.473075565D+03	-7.407474090D+01				

WO3- Gurvich, 1982 pt1 p51 pt2 p53.

2 tpi82 W	1.000	3.00E	1.00	0.00	0.00	0	231.8387486	-650475.961
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.630999684D+05	-1.967609682D+03	1.201970914D+01	1.681260779D-03	-5.859360060D-06				
5.028616330D-09	-1.434012198D-12		-7.009203990D+04	-3.936901040D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.637832510D+05	-1.347089334D+03	9.773637560D+00	1.071395459D-03	-3.842403660D-07				
5.737531900D-11	-3.157605982D-15		-7.239515570D+04	-2.391116343D+01				

(WO3)2 Gurvich, 1982 pt1 p52 pt2 p54.

2 tpi82 W	2.000	6.00	0.00	0.00	0.00	0	463.6764000	-1210443.298
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.088414510D+04	-9.060340790D+02	7.601575390D+00	5.241008510D-02	-7.922356390D-05				
5.708640180D-08	-1.606775042D-11		-1.441496996D+05	-1.093524051D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.674072430D+05	-7.032518360D+02	2.251617461D+01	-2.035473339D-04	4.444320340D-08				
-5.045188080D-12	2.318375739D-16		-1.502699479D+05	-8.613988980D+01				

(WO3)3 Gurvich, 1982 pt1 p53 pt2 p55.

2 tpi82 W	3.000	9.00	0.00	0.00	0.00	0	695.5146000	-2013291.101
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.485390010D+04	-1.933496319D+02	8.206544780D+00	8.599515510D-02	-1.257565252D-04				
8.891567220D-08	-2.471213564D-11		-2.462453469D+05	-5.657325260D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.450263310D+05	-1.133837222D+03	3.483479230D+01	-3.301361100D-04	7.226602130D-08				
-8.221581630D-12	3.785050840D-16		-2.488486308D+05	-1.441551053D+02				

(WO3)4 Gurvich, 1982 pt1 p54 pt2 p56.

2 tpi82 W	4.000	12.00	0.00	0.00	0.00	0	927.3528000	-2817433.885
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.388606167D+04	2.287518563D+02	8.662370000D+00	1.219700696D-01	-1.770499494D-04				
1.246790033D-07	-3.456182860D-11		-3.467839600D+05	-3.603937290D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.277530217D+06	-1.566538532D+03	4.715363520D+01	-4.563263220D-04	9.990758360D-08				
-1.136816181D-11	5.234399340D-16		-3.477418470D+05	-2.051588395D+02				

(WO3)5 Gurvich, 1982 pt1 p56 pt2 p57.

2 tpi82 W	5.000	15.00	0.00	0.00	0.00	0	1159.1910000	-3551492.326
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.497576743D+04	2.719999782D+02	1.138626896D+01	1.523302100D-01	-2.211447753D-04				
1.557377753D-07	-4.317244680D-11		-4.371424320D+05	-1.441643481D+01				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.600667953D+06	-1.958437864D+03	5.944227390D+01	-5.705105630D-04	1.249090916D-07				
-1.421320416D-11	6.544458260D-16		-4.384095860D+05	-2.660238838D+02				

Xe Ref-Elm. Moore, 1971. Moore, 1970a. Gordon, 1999.

3 g 1/99 XE	1.00	0.00	0.00	0.00	0.00	0	131.2930000	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-7.453750000D+02	6.164454205D+00				
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.025226680D+03	-1.209507521D+01	2.514153347D+00	-8.248102080D-06	2.530232618D-09				
-3.892333230D-13	2.360439138D-17		-6.685800730D+02	6.063710715D+00				
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.540397456D+08	-1.105373774D+05	1.382644099D+01	1.500614606D-03	-3.935359030D-07				
2.765790584D-11	-5.943990574D-16		9.285443830D+05	-1.109834556D+02				



## Appendix D (continued)

Xe+ Moore,1971. Moore,1970a. Gordon,1999.									
3 g 3/97 XE	1.00E	-1.00	0.00	0.00	0.00	0.00	0	131.2924514	1176552.232
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.002923620D+02	-1.218753648D+00	2.506016493D+00	-1.547411334D-05	2.191372741D-08					
-1.623684074D-11	4.929132670D-15		1.407665368D+05	7.516712465D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.241683887D+04	-1.500654643D+02	2.964678293D+00	-4.693396660D-04	1.959138719D-07					
-3.037761925D-11	1.637361082D-15		1.414966808D+05	4.565685735D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.562275878D+08	1.570476914D+05	-3.635537230D+01	5.019392580D-03	-3.438107240D-07					
1.140544651D-11	-1.295661530D-16		-1.103556546D+06	3.436188813D+02					
Zn Hf:Cox,1989. Sugar,1995. Gordon,1999.									
3 g 6/97 ZN	1.00	0.00	0.00	0.00	0.00	0	65.3900000	130400.000	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	2.500000000D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		1.493805072D+04	5.118861010D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.755591489D+05	4.984139240D+02	1.969386292D+00	2.608808787D-04	-5.627195080D-08					
2.723336049D-12	4.266685808D-16		1.173773458D+04	8.961085650D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.087287962D+08	1.578178131D+05	-3.622033110D+01	3.345230020D-03	-8.567422720D-09					
-7.122544740D-12	1.691187274D-16		-1.217847671D+06	3.459439960D+02					
Zn+ Sugar,1995. Gordon,1999.									
3 g 6/97 ZN	1.00E	-1.00	0.00	0.00	0.00	0	65.3894514	1043000.128	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.098344940D-04	-4.343581620D-06	2.500000019D+00	-4.389036810D-11	5.563969200D-14					
-3.638228260D-17	9.607881995D-21		1.246979918D+05	5.811995500D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.436179460D+05	9.567355240D+02	1.511478952D+00	4.613467960D-04	-8.786800980D-08					
7.558567780D-13	1.168827311D-15		1.185321933D+05	1.300742670D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.011747676D+09	2.074729347D+06	-5.589526960D+02	7.501396440D-02	-5.136763100D-06					
1.741662147D-10	-2.323920111D-15		-1.609057856D+07	4.824788010D+03					
Zr Hf:Gurvich,1982. Moore,1971. Hackett,1986. Gordon,1999.									
3 g 1/98 ZR	1.00	0.00	0.00	0.00	0.00	0	91.2240000	599318.611	
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.715899960D+04	-9.435981740D+02	6.359756180D+00	-9.790119730D-04	-7.608224150D-06					
9.308717430D-09	-3.124675586D-12		7.588019470D+04	-1.665770522D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.006771840D+06	-1.566960605D+04	1.796982350D+01	-6.763409650D-03	1.733678968D-06					
-2.064699786D-10	9.334092610D-15		1.734636249D+05	-1.051117377D+02					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
5.207701380D+08	-2.825652444D+05	6.077054350D+01	-5.081211410D-03	2.345845819D-07					
-6.237212120D-12	8.010718759D-17		2.351487351D+06	-5.093183060D+02					
Zr+ Moore,1971. Moore,1970a. Gordon,1999.									
3 g 1/98 ZR	1.00E	-1.00	0.00	0.00	0.00	0	91.2234514	1246246.292	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.739842193D+05	-2.224598466D+03	1.400787829D+01	-2.378785396D-02	2.641058912D-05					
-1.442565487D-08	3.135982142D-12		1.598210714D+05	-5.816728810D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.298137160D+05	-2.017117556D+03	5.037498300D+00	-5.503371950D-04	1.023753499D-07					
-1.261537793D-11	7.092401042D-16		1.620884945D+05	-9.820640860D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.294818875D+07	1.860972745D+04	-1.661509984D+00	6.020341290D-04	-3.930742580D-08					
1.543806931D-12	-2.618341088D-17		4.907298890D+03	4.642130480D+01					
Zr- Hotop,1985. Gordon,1999.									
3 g 2/98 ZR	1.00E	1.00	0.00	0.00	0.00	0	91.2245486	552952.398	
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.046662367D+04	-8.074277210D+02	9.213006110D+00	-1.614342054D-02	1.908653551D-05					
-1.138888914D-08	2.745019116D-12		6.903034030D+04	-2.862644371D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
8.471861160D+04	3.175439340D+02	2.251491246D+00	1.018645389D-04	-2.285208242D-08					
2.647293502D-12	-1.235813604D-16		6.422337600D+04	1.081261057D+01					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.386641560D+05	3.768748730D+02	2.417088403D+00	9.411538660D-06	-5.824251210D-10					
1.866281342D-14	-2.423724320D-19		6.334701050D+04	9.677778690D+00					

## Appendix D (continued)

ZrN Chase,1998 p1620.

2 j 6/63 ZR	1.00N	1.00	0.00	0.00	0.00	0.00	0.00	105.2307000	713372.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.259109156D+04	-1.802590198D+02	3.130058377D+00	5.427709280D-03	-8.264614840D-06					
5.958438220D-09	-1.670274535D-12		8.578881490D+04	8.470724780D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.255790890D+04	-8.126796600D+01	4.559924400D+00	1.291161650D-05	5.203830770D-09					
-5.927436670D-13	2.731548854D-17		8.468648390D+04	1.493633264D+00					

ZrO Gurvich,1982 pt1 p118 pt2 p118.

3 tps82 ZR	1.000	1.00	0.00	0.00	0.00	0.00	0.00	107.2234000	83922.708
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.091761400D+05	8.652770090D+03	-5.294740150D+01	1.728961761D-01	-2.457230895D-04					
1.672135156D-07	-4.423012380D-11		-3.095129818D+04	3.132576719D+02					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.648098310D+05	3.442314470D+02	4.815779180D+00	-4.660633140D-04	2.140489079D-07					
-2.054364483D-11	4.084667760D-16		7.317340700D+03	1.502933548D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.343456923D+08	-7.851088360D+04	1.981614195D+01	-8.027211020D-04	2.522081797D-09					
7.959625600D-13	-1.684162816D-17		6.406670590D+05	-1.358472283D+02					

ZrO+ Gurvich,1982 pt1 p122 pt2 p120.

3 tps82 ZR	1.000	1.00E	-1.00	0.00	0.00	0.00	0.00	107.2228514	720614.114
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
1.032911549D+04	7.304661220D+01	2.606345299D+00	5.099300290D-03	-6.250338760D-06					
3.797460020D-09	-9.198416900D-13		8.533233780D+04	1.267311019D+01					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-4.937166560D+05	6.699900760D+02	4.575353470D+00	-6.923237900D-04	4.280600940D-07					
-7.547660220D-11	4.414279860D-15		8.018880660D+04	2.928943704D+00					
6000.000	20000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.389941590D+07	-2.084044161D+04	8.167126240D+00	-5.668596640D-05	-8.861355220D-09					
4.773106180D-13	-7.435660480D-18		2.554517908D+05	-3.127152387D+01					

ZrO2 Gurvich,1982 pt1 p125. Chase,1998 p1772 12/65.

2 g10/99 ZR	1.000	2.00	0.00	0.00	0.00	0.00	0.00	123.2228000	-317042.737
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
3.637649000D+04	-2.620658297D+02	3.692866870D+00	1.214524156D-02	-1.822445342D-05					
1.299215204D-08	-3.615900110D-12		-3.801990880D+04	8.290857600D+00					
1000.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
2.854363887D+06	-8.738589890D+03	1.621315114D+01	-4.417922830D-03	8.959096920D-07					
-4.054667110D-11	-2.147732083D-15		1.527510023D+04	-7.481995490D+01					

Ag(cr) Cubic. Ref-Elm. Cox,1989 p228.

1 coda89 AG	1.00	0.00	0.00	0.00	0.00	0.00	0.00	107.8682000	0.000
200.000	1235.0807	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-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) Liquid. Ref-Elm. Cox,1989 p228.

1 coda89 AG	1.00	0.00	0.00	0.00	0.00	0.00	0.00	107.8682000	0.000
1235.080	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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) Cubic. Ref-Elm. Cox,1989 p217.

1 coda89 AL	1.00	0.00	0.00	0.00	0.00	0.00	0.00	26.9815380	0.000
200.000	933.6107	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-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) Liquid. Ref-Elm. Cox,1989 p217.

1 coda89 AL	1.00	0.00	0.00	0.00	0.00	0.00	0.00	26.9815380	0.000
933.610	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	3.818625510D+00	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-9.576323160D+01	-1.752553420D+01					

ALBr3(cr) Monoclinic. Gurvich,1996a pt1 p187 pt2 p150.

1 tps96 AL	1.00BR	3.00	0.00	0.00	0.00	0.00	0.00	266.6935380	-511500.000
200.000	371.1607	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.907292099D+05	0.000000000D+00	2.665662652D+01	-8.326099820D-02	1.395828123D-04					
0.000000000D+00	0.000000000D+00		-6.763881140D+04	-1.126522667D+02					

ALBr3(L) Liquid. Gurvich,1996a pt1 p187 pt2 p150.

1 tps96 AL	1.00BR	3.00	0.00	0.00	0.00	0.00	0.00	266.6935380	-511500.000
371.160	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	1.503395871D+01	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-6.481402080D+04	-6.083617689D+01					

## Appendix D (continued)

ALCL3(cr) Monoclinic. Gurvich,1996a pt1 p172 pt2 p133.  
 1 tps96 AL 1.00CL 3.00 0.00 0.00 0.00 1 133.3405380 -705100.000  
 200.000 465.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16980.000  
 -2.605551108D+05 2.535762396D+03-1.248379067D+00 2.465425813D-02-8.048550150D-06  
 0.000000000D+00 0.000000000D+00 -1.007777032D+05 2.030375677D+01

ALCL3(L) Liquid. Gurvich,1996a pt1 p172 pt2 p133.  
 1 tps96 AL 1.00CL 3.00 0.00 0.00 0.00 2 133.3405380 -705100.000  
 465.700 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16980.000  
 0.000000000D+00 0.000000000D+00 1.509409454D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.559022460D+04-6.519014639D+01

ALF3(II) Hexagonal. Gurvich,1996a pt1 p156 pt2 p119.  
 2 tps96 AL 1.00F 3.00 0.00 0.00 0.00 1 83.9767476 -1510400.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11620.400  
 0.000000000D+00 0.000000000D+00-2.444621150D+00 6.248607440D-02-8.043962500D-05  
 0.000000000D+00 0.000000000D+00 -1.829961207D+05 6.871585170D+00  
 298.150 728.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11620.400  
 0.000000000D+00 0.000000000D+00-3.158574588D+00 7.101368571D-02-1.246540085D-04  
 7.930377136D-08 0.000000000D+00 -1.829283321D+05 9.661469435D+00

ALF3(I) Cubic. Gurvich,1996a pt1 p156 pt2 p119.  
 1 tps96 AL 1.00F 3.00 0.00 0.00 0.00 2 83.9767476 -1510400.000  
 728.000 2100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11620.400  
 -1.060675855D+05 0.000000000D+00 1.114052422D+01 1.092668119D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.853502219D+05-5.651122021D+01

ALH3(a) Alpha,hexagonal. Gurvich,1996a pt1 p144 pt2 p108.  
 1 tps96 AL 1.00H 3.00 0.00 0.00 0.00 1 30.0053580 -11400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5440.000  
 5.744612990D+05-7.649579650D+03 3.481355430D+01-4.495737990D-02 2.948551342D-05  
 0.000000000D+00 0.000000000D+00 3.549793150D+04-2.050727589D+02

ALI3(cr) Hexagonal. Gurvich,1996a pt1 p193 pt2 p155.  
 1 tps96 AL 1.00I 3.00 0.00 0.00 0.00 1 407.6949480 -302900.000  
 298.150 461.4707 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22300.000  
 -3.486280460D+03 0.000000000D+00 8.644374370D+00 1.088065032D-02 5.040262220D-07  
 0.000000000D+00 0.000000000D+00 -3.950736400D+04-2.968661932D+01

ALI3(L) Liquid. Gurvich,1996a pt1 p193 pt2 p155.  
 1 tps96 AL 1.00I 3.00 0.00 0.00 0.00 2 407.6949480 -302900.000  
 461.470 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22300.000  
 0.000000000D+00 0.000000000D+00 1.455287203D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.913903150D+04-5.670488781D+01

ALN(cr) Hexagonal. Gurvich,1996a pt1 p202 pt2 p163.  
 2 tps96 AL 1.00N 1.00 0.00 0.00 0.00 1 40.9882380 -319000.000  
 100.000 300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 3870.000  
 3.654741530D+03 0.000000000D+00-2.148600451D+00 2.744441314D-02-2.763366825D-05  
 0.000000000D+00 0.000000000D+00 -3.868948290D+04 7.733969220D+00  
 300.000 1800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 3870.000  
 -1.801549340D+05 0.000000000D+00 5.525280504D+00 4.025492783D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.063616530D+04-3.018829926D+01

ALN(L) Liquid. Gurvich,1996a pt1 p202 pt2 p163.  
 2 tps96 AL 1.00N 1.00 0.00 0.00 0.00 3 40.9882380 -319000.000  
 1800.000 2700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 3870.000  
 0.000000000D+00 0.000000000D+00 4.491184688D+00 9.460569534D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.955518910D+04-2.338770283D+01  
 2700.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 3870.000  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.755928440D+04-4.598731266D+01

AL(OH)3(a) Gibbsite. Gurvich,1996a pt1 p150 pt2 p114.  
 1 tps96 AL 1.00O 3.00H 3.00 0.00 0.00 1 78.0035580 -1293500.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12460.000  
 -2.376748819D+04 9.289791210D+02-1.532337335D+01 1.307578268D-01-2.205157141D-04  
 1.567014467D-07 0.000000000D+00 -1.605485750D+05 6.795129010D+01

AL2O3(a) Alpha,corundum. Gurvich,1996a pt1 p134 pt2 p103.  
 3 tps96 AL 2.00O 3.00 0.00 0.00 0.00 1 101.9612760 -1675700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10016.000  
 -5.391549970D+06 1.036676983D+05-8.173229150D+02 3.388258720D+00-7.512400360D-03  
 8.659248820D-06-4.066085670D-09 -6.660134650D+05 4.235502230D+03  
 500.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10016.000  
 -6.042087868D+05 0.000000000D+00 1.475480816D+01 8.272285438D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.079235447D+05-8.136029480D+01  
 1200.000 2327.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10016.000  
 0.000000000D+00 0.000000000D+00 1.293774378D+01 1.992781294D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.060787581D+05-6.966603728D+01

## Appendix D (continued)

AL2O3(L) Liquid. Gurvich,1996a pt1 p134 pt2 p103.  
1 tps96 AL 2.000 3.00 0.00 0.00 0.00 3 101.9612760 -1675700.000  
2327.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10016.000  
0.000000000D+00 0.000000000D+00 1.959225499D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -2.027701571D+05-1.108590952D+02

AL2S3(a) Hexagonal alpha. Gurvich,1996a pt1 p201 pt2 p162.  
2 tps96 AL 2.00S 3.00 0.00 0.00 0.00 1 150.1580760 -648500.000  
100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18630.440  
0.000000000D+00 0.000000000D+00-1.347810098D+00 8.478152110D-02-1.270516814D-04  
0.000000000D+00 0.000000000D+00 -8.024014680D+04 2.103644584D+00  
298.150 1273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18630.440  
-1.943109095D+05 0.000000000D+00 1.417618116D+01 2.164890054D-03 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -8.297075040D+04-6.845362098D+01

AL2S3(b) Rhombohedral gamma. Gurvich,1996a pt1 p201 pt2 p162.  
1 tps96 AL 2.00S 3.00 0.00 0.00 0.00 3 150.1580760 -648500.000  
1273.000 1373.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18630.440  
0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -8.445251510D+04-8.466769750D+01

AL2S3(L) Liquid. Gurvich,1996a pt1 p201 pt2 p162.  
1 tps96 AL 2.00S 3.00 0.00 0.00 0.00 4 150.1580760 -648500.000  
1373.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18630.440  
0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -8.114023330D+04-9.722848599D+01

AL2SiO5(an) Andalusite. Chase,1998 p160.  
3 j 9/67 AL 2.00SI 1.000 5.00 0.00 0.00 1 162.0455760 -2592072.000  
200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17093.000  
-5.435020350D+05 8.364904470D+03-5.479541870D+01 2.421451459D-01-3.247828060D-04  
1.619746222D-07 0.000000000D+00 -3.531115760D+05 2.892220103D+02  
600.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17093.000  
9.635670330D+06-6.505315100D+04 1.886717981D+02-2.227599181D-01 1.677460173D-04  
-6.532301110D-08 1.041420443D-11 4.284683500D+04-1.170130476D+03  
1500.000 3000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17093.000  
5.600590290D+07-1.591905491D+05 2.058003747D+02-1.103017260D-01 3.860284650D-05  
-6.943079960D-09 5.126291370D-13 6.964365160D+05-1.424396263D+03

AL4C3(cr) Hexagonal. Gurvich,1996a pt1 p207 pt2 p168.  
2 tps96 AL 4.00C 3.00 0.00 0.00 0.00 1 143.9582520 -206900.000  
100.000 300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16470.000  
4.384127580D+03 0.000000000D+00-5.803779650D+00 1.009595640D-01-1.158851541D-04  
0.000000000D+00 0.000000000D+00 -2.660263745D+04 1.884004031D+01  
300.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16470.000  
-4.483607573D+05 0.000000000D+00 1.788920814D+01 4.024290066D-03 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -3.190056250D+04-9.494910735D+01

B(b) Beta. Ref-Elm. Chase,1998 p177-180. McBride,1993a.  
2 j 6/83 B 1.00 0.00 0.00 0.00 0.00 1 10.8110000 0.000  
200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 1214.000  
2.598259342D+05-4.770773050D+03 3.464124480D+01-1.287342209D-01 2.897864235D-04  
-3.307265950D-07 1.500151011D-10 2.146946846D+04-1.830824723D+02  
600.000 2350.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 1214.000  
-8.697700220D+02-8.050405960D+02 4.079712880D+00-6.423381350D-04 4.846017800D-07  
-1.252780673D-10 1.335923595D-14 3.397919930D+03-2.505906587D+01

B(L) Liquid. Ref-Elm. Chase,1998 p177-180. McBride,1993a.  
1 j 6/83 B 1.00 0.00 0.00 0.00 0.00 2 10.8110000 0.000  
2350.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 1214.000  
0.000000000D+00 0.000000000D+00 3.818625511D+00 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 3.360603140D+03-2.073167308D+01

BN(cr) Hexagonal. Gurvich,1996a pt1 p103 pt2 p82.  
2 tps96 B 1.00N 1.00 0.00 0.00 0.00 1 24.8177000 -251000.000  
200.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 2628.425  
4.927312430D+05-6.086406850D+03 2.678226753D+01-4.529686640D-02 5.305526030D-05  
-3.041114432D-08 6.795343860D-12 -2.413474891D+02-1.570534002D+02  
1200.000 3240.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 2628.425  
-8.394039490D+05 0.000000000D+00 6.231256640D+00-1.258688680D-05 2.018144787D-09  
0.000000000D+00 0.000000000D+00 -3.427269230D+04-3.687260910D+01

BN(L) Liquid. Gurvich,1996a pt1 p103 pt2 p82.  
1 tps96 B 1.00N 1.00 0.0

## Appendix D (continued)

B2O3(cr) Hexagonal. Gurvich,1996a pt1 p21 pt2 p16.  
 1 tpis96 B 2.000 3.00 0.00 0.00 0.00 0.00 1 69.6202000 -1273500.000  
 100.000 723.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9301.499  
 -5.595297380D+04 1.311214190D+03-1.178535942D+01 7.702795250D-02-9.740126500D-05  
 4.692119720D-08 1.804813810D-12 -1.599672923D+05 5.866759160D+01

B2O3(L) Liquid. Gurvich,1996a pt1 p21 pt2 p16.  
 1 tpis96 B 2.000 3.00 0.00 0.00 0.00 0.00 2 69.6202000 -1273500.000  
 723.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9301.499  
 3.774124994D+05 0.000000000D+00 1.528015481D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.562115789D+05-8.056094941D+01

B2S3(cr) Monoclinic. Gurvich,1996a pt1 p101 pt2 p80.  
 1 tpis96 B 2.00S 3.00 0.00 0.00 0.00 1 117.8170000 -243000.000  
 298.150 840.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17200.400  
 -9.430501617D+04 0.000000000D+00 1.190088171D+01 8.711277033D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.347775180D+04-5.890696350D+01

B2S3(L) Liquid. Gurvich,1996a pt1 p101 pt2 p80.  
 1 tpis96 B 2.00S 3.00 0.00 0.00 0.00 2 117.8170000 -243000.000  
 840.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17200.400  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.921234633D+04-8.268126136D+01

B3O3H3(cr) Chase,1998 p287.  
 3 j 3/65 B 3.00H 3.000 3.00 0.00 0.00 1 83.4550200 -1262313.000  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -5.328545240D+05 3.767360370D+03 6.890276350D-01-4.217091030D-03 8.303566290D-05  
 -6.146021890D-08 0.000000000D+00 -1.757027581D+05 2.395113516D+01  
 700.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 5.084004120D+07-3.177180280D+05 8.113753320D+02-1.045412717D+00 7.976442970D-04  
 -3.265400500D-07 5.554759650D-11 1.623716865D+06-5.113032450D+03  
 1400.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -3.234845810D+08 1.232060747D+06-1.920881017D+03 1.628142178D+00-7.579315580D-04  
 1.870131216D-07-1.915685535D-11 -7.655560210D+06 1.307505171D+04

B4C(cr) Hexagonal. Gurvich,1996a pt1 p111 pt2 p89  
 2 tpis96 B 4.00C 1.00 0.00 0.00 0.00 1 55.2547000 -62000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5611.469  
 -3.582115390D+07 6.748884130D+05-5.160630080D+03 2.049973510D+01-4.453648770D-02  
 5.049831300D-05-2.340979136D-08 -3.040618105D+06 2.693617477D+04  
 500.000 2743.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5611.469  
 -5.772904970D+05 0.000000000D+00 1.274373364D+01 5.718209610D-05 1.287030822D-06  
 0.000000000D+00 0.000000000D+00 -1.320621763D+04-7.266962500D+01

B4C(L) Liquid. Chase,1998 pp556-8.  
 1 j 6/83 B 4.00C 1.00 0.00 0.00 0.00 2 55.2547000 -62000.000  
 2743.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5611.469  
 0.000000000D+00 0.000000000D+00 1.635454164D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.250553215D+03-9.163227046D+01

Ba(cr) Crystal. Ref-Elm. Alcock,1993.  
 2 srd 93 BA 1.00 0.00 0.00 0.00 0.00 1 137.3270000 0.000  
 80.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6906.992  
 -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 2 137.3270000 0.000  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6906.992  
 0.000000000D+00 0.000000000D+00 4.810866786D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.920623810D+02-2.000275711D+01

BaBr2(cr) Rhombic. Gurvich,1996a pt1 p578 pt2 p438.  
 1 tpis96 BA 1.00BR 2.00 0.00 0.00 0.00 1 297.1350000 -752000.000  
 298.000 1130.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19000.460  
 -7.817658527D+03 0.000000000D+00 8.433088661D+00 2.644894287D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.310239840D+04-3.084013513D+01

BaBr2(L) Liquid. Gurvich,1996a pt1 p578 pt2 p438.  
 1 tpis96 BA 1.00BR 2.00 0.00 0.00 0.00 2 297.1350000 -752000.000  
 1130.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19000.460  
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.227494300D+04-5.391493900D+01

## Appendix D (continued)

BaCO<sub>3</sub>(a) CrIII,rhombic. Gurvich,1996a pt1 p588 pt2 p446.  
 2 tps96 BA 1.00C 1.000 3.00 0.00 0.00 1 197.3359000 -1214000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16510.460  
 -2.877181104D+07 5.413510470D+05-4.125297560D+03 1.638620098D+01-3.558188760D-02  
 4.031953330D-05-1.867325900D-08 -2.581769925D+06 2.154826876D+04  
 500.000 1083.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16510.460  
 -4.578261377D+05 0.000000000D+00 1.897622349D+01-1.614166078D-02 1.493894409D-05  
 0.000000000D+00 0.000000000D+00 -1.526176829D+05-9.306389650D+01

BaCO<sub>3</sub>(b) CrII,hexagonal. Gurvich,1996a pt1 p588 pt2 p446.  
 1 tps96 BA 1.00C 1.000 3.00 0.00 0.00 3 197.3359000 -1214000.000  
 1083.000 1233.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16510.460  
 0.000000000D+00 0.000000000D+00 1.900292380D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.534042929D+05-9.996568172D+01

BaCO<sub>3</sub>(c) CrI,cubic. Gurvich,1996a pt1 p588 pt2 p446.  
 1 tps96 BA 1.00C 1.000 3.00 0.00 0.00 4 197.3359000 -1214000.000  
 1233.000 1828.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16510.460  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.533520950D+05-1.013948007D+02

BaCO<sub>3</sub>(L) Liquid. Gurvich,1996a pt1 p588 pt2 p446.  
 1 tps96 BA 1.00C 1.000 3.00 0.00 0.00 5 197.3359000 -1214000.000  
 1828.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16510.460  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.496405113D+05-1.032798247D+02

BaCL<sub>2</sub>(a) CrII,rhombic. Gurvich,1996a pt1 p574 pt2 p435.  
 2 tps96 BA 1.00CL 2.00 0.00 0.00 0.00 1 208.2330000 -855200.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16700.460  
 -7.376444120D+04 1.806760784D+03-1.415837573D+01 1.391571933D-01-4.179089240D-04  
 6.207438290D-07-3.577305500D-10 -1.127273901D+05 7.349900590D+01  
 500.000 1198.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16700.460  
 7.096028509D+02 0.000000000D+00 8.343245723D+00 2.300676769D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.054434434D+05-3.333989736D+01

BaCL<sub>2</sub>(b) CrI,cubic. Gurvich,1996a pt1 p574 pt2 p435.  
 1 tps96 BA 1.00CL 2.00 0.00 0.00 0.00 3 208.2330000 -855200.000  
 1198.000 1234.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16700.460  
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.105803253D+05-8.137880037D+01

BaCL<sub>2</sub>(L) Liquid. Gurvich,1996a pt1 p574 pt2 p435.  
 1 tps96 BA 1.00CL 2.00 0.00 0.00 0.00 4 208.2330000 -855200.000  
 1234.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16700.460  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.054088841D+05-6.099987667D+01

BaF<sub>2</sub>(a) CrIII,cubic. Gurvich,1996a pt1 p567 pt2 p431.  
 2 tps96 BA 1.00F 2.00 0.00 0.00 0.00 1 175.3238064 -1206000.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14440.460  
 1.441693954D+05-4.606283760D+03 5.412180390D+01-2.221460987D-01 5.733095130D-04  
 -7.321844990D-07 3.715051400D-10 -1.283756240D+05-2.649277473D+02  
 500.000 1240.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14440.460  
 -2.180525371D+04 0.000000000D+00 7.730461567D+00 3.587703906D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.475854552D+05-3.364924914D+01

BaF<sub>2</sub>(b) CrII. Gurvich,1996a pt1 p567 pt2 p431.  
 1 tps96 BA 1.00F 2.00 0.00 0.00 0.00 3 175.3238064 -1206000.000  
 1240.000 1480.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14440.460  
 0.000000000D+00 0.000000000D+00 1.515423038D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.533548254D+05-8.153942783D+01

BaF<sub>2</sub>(c) CrI. Gurvich,1996a pt1 p567 pt2 p431.  
 1 tps96 BA 1.00F 2.00 0.00 0.00 0.00 4 175.3238064 -1206000.000  
 1480.000 1641.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14440.460  
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.535821388D+05-8.396607945D+01

BaF<sub>2</sub>(L) Liquid. Gurvich,1996a pt1 p567 pt2 p431.  
 1 tps96 BA 1.00F 2.00 0.00 0.00 0.00 5 175.3238064 -1206000.000  
 1641.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14440.460  
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.467045237D+05-6.129240287D+01

BaH<sub>2</sub>(a) CrII,rhombic Gurvich,1996a pt1 p556 pt2 p424.  
 1 tps96 BA 1.00H 2.00 0.00 0.00 0.00 1 139.3428800 -190000.000  
 298.150 871.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9100.474  
 0.000000000D+00 0.000000000D+00 4.530874339D+00 3.359308005D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.435180761D+04-1.923955725D+01

## Appendix D (continued)

BaH2(b) CrI, rhombic Gurvich, 1996a pt1 p556 pt2 p424.  
 1 tps96 BA 1.00H 2.00 0.00 0.00 0.00 2 139.3428800 -190000.000  
 871.000 1473.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9100.474  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.589536064D+04 -4.267585539D+01

BaH2(L) Liquid Gurvich, 1996a pt1 p556 pt2 p424.  
 1 tps96 BA 1.00H 2.00 0.00 0.00 0.00 3 139.3428800 -190000.000  
 1473.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9100.474  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.359720958D+04 -4.414413915D+01

BaI2(cr) Rhombic. Gurvich, 1996a pt1 p582 pt2 p441.  
 2 tps96 BA 1.00I 2.00 0.00 0.00 0.00 1 391.1359400 -606000.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19230.400  
 1.510332529D+04 -6.224807000D+02 1.545037842D+01 -3.239437030D-02 9.253598890D-05  
 -1.251913725D-07 6.804559110D-11 -7.305629580D+04 -6.364696150D+01  
 500.000 984.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19230.400  
 -3.247335080D+02 0.000000000D+00 8.607723125D+00 2.399780624D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.555873070D+04 -2.989160688D+01

BaI2(L) Liquid. Gurvich, 1996a pt1 p582 pt2 p441.  
 1 tps96 BA 1.00I 2.00 0.00 0.00 0.00 3 391.1359400 -606000.000  
 984.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19230.400  
 0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.611264840D+04 -5.863183475D+01

BaO(cr) Cubic Gurvich, 1996a pt1 p547 pt2 p418.  
 3 tps96 BA 1.00O 1.00 0.00 0.00 0.00 1 153.3264000 -548000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9962.459  
 -3.734308680D+06 7.030482670D+04 -5.334141930D+02 2.143135900D+00 -4.664219600D-03  
 5.294704440D-06 -2.456512761D-09 -3.833163320D+05 2.789047565D+03  
 500.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9962.459  
 -7.551858137D+04 0.000000000D+00 6.798957485D+00 -1.205482945D-03 7.325747398D-07  
 0.000000000D+00 0.000000000D+00 -6.814216420D+04 -3.017618534D+01  
 1400.000 2246.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9962.459  
 1.380021192D+07 0.000000000D+00 -1.685992319D+01 1.166250326D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.704906000D+04 1.274565988D+02

BaO(L) Liquid Gurvich, 1996a pt1 p547 pt2 p418.  
 1 tps96 BA 1.00O 1.00 0.00 0.00 0.00 3 153.3264000 -548000.000  
 2246.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9962.459  
 0.000000000D+00 0.000000000D+00 1.001863008D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.861430250D+04 -5.267326797D+01

Ba(OH)2(b) CrII, rhombic Gurvich, 1996a pt1 p558 pt2 p427.  
 1 tps96 BA 1.00O 2.00H 2.00 0.00 0.00 1 171.3416800 -940600.000  
 100.000 519.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16148.440  
 5.078717800D+04 -1.641996937D+03 1.964278489D+01 -3.730614630D-02 1.039952734D-04  
 -8.659369050D-08 2.282290989D-11 -1.085585521D+05 -9.701503650D+01

Ba(OH)2(a) CrI, rhombic Gurvich, 1996a pt1 p558 pt2 p427.  
 1 tps96 BA 1.00O 2.00H 2.00 0.00 0.00 2 171.3416800 -940600.000  
 519.000 681.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16148.440  
 0.000000000D+00 0.000000000D+00 1.491368704D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.176117467D+05 -7.252241184D+01

Ba(OH)2(L) Liquid Gurvich, 1996a pt1 p558 pt2 p427.  
 1 tps96 BA 1.00O 2.00H 2.00 0.00 0.00 3 171.3416800 -940600.000  
 681.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16148.440  
 0.000000000D+00 0.000000000D+00 1.659749041D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.168340700D+05 -8.068104197D+01

BaS(cr) Cubic. Gurvich, 1996a pt1 p584 pt2 p443.  
 2 tps96 BA 1.00S 1.00 0.00 0.00 0.00 1 169.3920000 -470000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10820.450  
 3.369786470D+05 -6.138740230D+03 4.922553770D+01 -1.599274620D-01 3.314481350D-04  
 -3.600847800D-07 1.611281388D-10 -3.028248993D+04 -2.539125160D+02  
 500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10820.450  
 -2.050631967D+04 0.000000000D+00 5.920852822D+00 8.307164223D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.839868930D+04 -2.466233780D+01

BaS(L) Liquid. Gurvich, 1996a pt1 p584 pt2 p443.  
 1 tps96 BA 1.00S 1.00 0.00 0.00 0.00 3 169.3920000 -470000.000  
 2500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10820.450  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.356075540D+04 -3.627577743D+01

## Appendix D (continued)

BaSO<sub>4</sub>(a) CrII, rhombic. Gurvich, 1996a pt1 p587 pt2 p445.  
 2 tps96 BA 1.00S 1.000 4.00 0.00 0.00 1 233.3896000 -1470000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19180.440  
 -1.712286968D+07 3.212789860D+05 -2.441820133D+03 9.713067900D+00 -2.105021811D-02  
 2.383101570D-05 -1.103328957D-08 -1.624343960D+06 1.276058048D+04  
 500.000 1423.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19180.440  
 -2.747004935D+05 0.000000000D+00 1.352094110D+01 6.200004570D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.820275447D+05 -6.454315519D+01

BaSO<sub>4</sub>(b) CrI, cubic. Gurvich, 1996a pt1 p587 pt2 p445.  
 1 tps96 BA 1.00S 1.000 4.00 0.00 0.00 3 233.3896000 -1470000.000  
 1423.000 1853.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19180.440  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.842091207D+05 -1.050884025D+02

BaSO<sub>4</sub>(L) Liquid. Gurvich, 1996a pt1 p587 pt2 p435.  
 1 tps96 BA 1.00S 1.000 4.00 0.00 0.00 4 233.3896000 -1470000.000  
 1853.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19180.440  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.793982539D+05 -1.024921441D+02

Be(a) Alpha. Ref-Elm. Alcock, 1993.  
 2 srd 93 BE 1.00 0.00 0.00 0.00 0.00 1 9.0121820 0.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 1942.068  
 3.532378938D+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 9.0121820 0.000  
 1543.000 1563.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 1942.068  
 0.000000000D+00 0.000000000D+00 3.608150089D+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 9.0121820 0.000  
 1563.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 1942.068  
 0.000000000D+00 0.000000000D+00 3.545608821D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.074755804D+02 -1.895341257D+01

BeAL2O<sub>4</sub>(cr) Chase, 1998 pp139-41.  
 3 j12/79 BE 1.00AL 2.000 4.00 0.00 0.00 1 126.9728580 -2300782.000  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13088.000  
 5.671733300D+05 -8.864346630D+03 4.407635150D+01 -3.612460380D-02 3.491655240D-05  
 -1.451255323D-08 0.000000000D+00 -2.361266575D+05 -2.603504873D+02  
 600.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13088.000  
 3.035781649D+07 -2.195328809D+05 6.571002230D+02 -9.751675120D-01 8.342636270D-04  
 -3.757959390D-07 6.972665420D-11 9.154378130D+05 -4.048262870D+03  
 1200.000 2146.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13088.000  
 5.346540420D+06 -2.333165977D+04 6.465121650D+01 -5.623102150D-02 4.944443190D-05  
 -2.347465372D-08 4.584679740D-12 -1.453507980D+05 -3.997587750D+02

BeAL2O<sub>4</sub>(L) Chase, 1998 pp139-41.  
 1 j12/79 BE 1.00AL 2.000 4.00 0.00 0.00 2 126.9728580 -2300782.000  
 2146.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13088.000  
 0.000000000D+00 0.000000000D+00 2.963602185D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.805665995D+05 -1.711673740D+02

BeBr<sub>2</sub>(cr) Cr, rhombic. Gurvich, 1996a pt1 p376 pt2 p301.  
 1 tps96 BE 1.00BR 2.00 0.00 0.00 0.00 1 168.8201820 -358000.000  
 298.150 781.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14900.000  
 -1.296528599D+05 0.000000000D+00 9.544519160D+00 8.967455689D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.637767130D+04 -4.238810553D+01

BeBr<sub>2</sub>(L) Liquid. Gurvich, 1996a pt1 p376 pt2 p301.  
 1 tps96 BE 1.00BR 2.00 0.00 0.00 0.00 2 168.8201820 -358000.000  
 781.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14900.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.571223050D+04 -5.534538359D+01

BeCO<sub>3</sub>(cr) Gurvich, 1996a pt1 p385 pt2 p310.  
 1 tps96 BE 1.00C 1.000 3.00 0.00 0.00 1 69.0210820 -1045000.000  
 298.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9200.480  
 -3.688732108D+05 0.000000000D+00 1.057428520D+01 4.670148932D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.302813975D+05 -5.746109667D+01



## Appendix D (continued)

BeCL2(a) Cr, rhombic. Gurvich, 1996a pt1 p370 pt2 p296.  
 1 tpis96 BE 1.00CL 2.00 0.00 0.00 0.00 1 79.9181820 -496200.000  
 200.000 676.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11420.000  
 -9.696336540D+05 1.653841300D+04 -1.120322868D+02 4.343457410D-01 -8.234422230D-04  
 7.967601960D-07 -3.089202126D-10 -1.372167152D+05 5.981191760D+02

BeCL2(b) CrI. Gurvich, 1996a pt1 p370 pt2 p296.  
 1 tpis96 BE 1.00CL 2.00 0.00 0.00 0.00 2 79.9181820 -496200.000  
 676.000 688.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11420.000  
 0.000000000D+00 0.000000000D+00 8.056999150D+00 2.516083329D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.169505530D+04 -3.701517264D+01

BeCL2(L) Liquid. Gurvich, 1996a pt1 p370 pt2 p296.  
 1 tpis96 BE 1.00CL 2.00 0.00 0.00 0.00 3 79.9181820 -496200.000  
 688.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11420.000  
 0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.212751630D+04 -5.342382325D+01

BeF2(a) CrII, hexagonal. Gurvich, 1996a pt1 p364 pt2 p292.  
 1 tpis96 BE 1.00F 2.00 0.00 0.00 0.00 1 47.0089884 -1027000.000  
 200.000 493.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8468.000  
 3.082582728D+05 -5.000745390D+03 3.049066381D+01 -5.416146720D-02 5.846680620D-05  
 0.000000000D+00 0.000000000D+00 -1.011928897D+05 -1.687961461D+02

BeF2(b) CrI, hexagonal. Gurvich, 1996a pt1 p364 pt2 p292.  
 1 tpis96 BE 1.00F 2.00 0.00 0.00 0.00 2 47.0089884 -1027000.000  
 493.000 823.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8468.000  
 0.000000000D+00 0.000000000D+00 5.652527930D+00 3.986885577D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.252903029D+05 -2.679700109D+01

BeF2(L) Liquid. Gurvich, 1996a pt1 p364 pt2 p292.  
 1 tpis96 BE 1.00F 2.00 0.00 0.00 0.00 3 47.0089884 -1027000.000  
 823.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8468.000  
 -1.882035141D+06 0.000000000D+00 1.234468417D+01 -1.836548396D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.310986361D+05 -6.898102574D+01

BeI2(cr) Cr, rhombic. Gurvich, 1996a pt1 p379 pt2 p304.  
 1 tpis96 BE 1.00I 2.00 0.00 0.00 0.00 1 262.8211220 -191000.000  
 298.150 763.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15200.000  
 -1.443741122D+05 0.000000000D+00 1.007828483D+01 3.371214900D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.647594661D+04 -4.378170625D+01

BeI2(L) Liquid. Gurvich, 1996a pt1 p379 pt2 p304.  
 1 tpis96 BE 1.00I 2.00 0.00 0.00 0.00 2 262.8211220 -191000.000  
 763.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15200.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.551070377D+04 -5.349837990D+01

BeO(a) CrII, hexagonal. Gurvich, 1996a pt1 p348 pt2 p278.  
 2 tpis96 BE 1.00O 1.00 0.00 0.00 0.00 1 25.0115820 -609400.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 2837.000  
 2.047701543D+05 -2.981173217D+03 1.385643338D+01 -1.581697711D-02 2.353849388D-05  
 -1.941029834D-08 6.520569610D-12 -5.922219190D+04 -8.231113660D+01  
 1000.000 2373.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 2837.000  
 1.024057237D+06 1.937465590D+03 -2.170213872D+00 6.700940070D-03 -1.829092628D-06  
 2.757893870D-10 -2.712743027D-14 -8.276808970D+04 1.896607400D+01

BeO(b) CrI, tetragonal. Gurvich, 1996a pt1 p348 pt2 p278.  
 1 tpis96 BE 1.00O 1.00 0.00 0.00 0.00 2 25.0115820 -609400.000  
 2373.000 2851.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 2837.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.674474850D+04 -3.937528813D+01

BeO(L) Liquid. Gurvich, 1996a pt1 p348 pt2 p278.  
 1 tpis96 BE 1.00O 1.00 0.00 0.00 0.00 3 25.0115820 -609400.000  
 2851.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 2837.000  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.600243170D+04 -6.253805395D+01

Be(OH)2(b) Rhombic, beta. Gurvich, 1996a pt1 p359 pt2 p289.  
 2 tpis96 BE 1.00O 2.00H 2.00 0.00 0.00 1 43.0268620 -905700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8293.440  
 -2.821507074D+07 5.306026240D+05 -4.050124700D+03 1.608285663D+01 -3.491136410D-02  
 3.956008990D-05 -1.833019806D-08 -2.495097922D+06 2.114570392D+04  
 500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8293.440  
 -4.549275904D+05 0.000000000D+00 1.198362862D+01 2.034996650D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.141192354D+05 -6.597431876D+01

BeS(cr) Cr, cubic. Gurvich, 1996a pt1 p381 pt2 p306.  
 1 tpis96 BE 1.00S 1.00 0.00 0.00 0.00 1 41.0771820 -236000.000  
 298.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5500.480  
 -1.061156941D+05 0.000000000D+00 4.876054031D+00 1.363880734D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.025444334D+04 -2.469606404D+01

## Appendix D (continued)

BeSO<sub>4</sub>(a) CrIII,tetr. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tps96 BE 1.00S 1.000 4.00 0.00 0.00 1 105.0747820 -1200000.000  
 200.000 861.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12970.000  
 9.674052850D+05-1.525976877D+04 9.078019340D+01-2.151323890D-01 3.405813330D-04  
 -2.623119799D-07 8.137303080D-11 -7.417050650D+04-5.024380540D+02

BeSO<sub>4</sub>(b) CrII,rhombic. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tps96 BE 1.00S 1.000 4.00 0.00 0.00 2 105.0747820 -1200000.000  
 861.000 912.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12970.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.508085273D+05-9.670719282D+01

BeSO<sub>4</sub>(c) CrI,cubic. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tps96 BE 1.00S 1.000 4.00 0.00 0.00 3 105.0747820 -1200000.000  
 912.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12970.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.505559568D+05-9.643025148D+01

BeSO<sub>4</sub>(L) Liquid. Gurvich,1996a pt1 p383 pt2 p308.  
 1 tps96 BE 1.00S 1.000 4.00 0.00 0.00 4 105.0747820 -1200000.000  
 1400.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12970.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.498343268D+05-9.591480146D+01

Be<sub>2</sub>C(cr) Barin,1989. Barin,1973.  
 1 bar 89 BE 2.00C 1.00 0.00 0.00 0.00 1 30.0350640 -116984.640  
 298.150 2400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 4.437364559D+00 2.569424296D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.550714068D+04-2.408584259D+01

Be<sub>2</sub>C(L) Barin,1989. Barin,1973.  
 1 bar 89 BE 2.00C 1.00 0.00 0.00 0.00 2 30.0350640 -116984.640  
 2400.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 1.107076665D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.496946374D+04-6.577435374D+01

Be<sub>3</sub>N<sub>2</sub>(a) CrII,cubic. Gurvich,1996a pt1 p384 pt2 p309.  
 2 tps96 BE 3.00N 2.00 0.00 0.00 0.00 1 55.0499460 -588000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7124.000  
 6.443341310D+05-9.239880870D+03 4.211333200D+01-4.513325350D-02 3.232975930D-05  
 0.000000000D+00 0.000000000D+00 -2.674920290D+04-2.511544265D+02  
 500.000 1673.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7124.000  
 -2.278465381D+05 4.432191420D+02 1.376274664D+00 3.225384830D-02-2.704770612D-05  
 8.116575420D-09-6.682374890D-14 -7.562743780D+04-1.197625563D+01

Be<sub>3</sub>N<sub>2</sub>(b) CrI,hexagonal. Gurvich,1996a pt1 p384 pt2 p309.  
 1 tps96 BE 3.00N 2.00 0.00 0.00 0.00 2 55.0499460 -588000.000  
 1673.000 2473.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7124.000  
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.850942150D+04-1.016302777D+02

Be<sub>3</sub>N<sub>2</sub>(L) Liquid. Gurvich,1996a pt1 p384 pt2 p309.  
 1 tps96 BE 3.00N 2.00 0.00 0.00 0.00 3 55.0499460 -588000.000  
 2473.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7124.000  
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.182303830D+04-1.169540588D+02

Br<sub>2</sub>(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 1 159.8080000 0.000  
 200.000 265.9007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24520.000  
 -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

Br<sub>2</sub>(L) Liq.Ref-Elm.Gurvich,1989 pt2 p314.Chase,1998 p471(6/82).  
 2 g 8/01 BR 2.00 0.00 0.00 0.00 0.00 2 159.8080000 0.000  
 265.900 332.5037 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24520.000  
 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

## Appendix D (continued)

C(gr) Graphite. Ref-Elm. TRC(4/83) vc,uc,tc1000-1002.									
3 n 4/83 C	1.00	0.00	0.00	0.00	0.00	1	12.0107000	0.000	
200.000	600.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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
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
2.023105106D+05	-1.138235908D+03	3.700279500D+00	-1.833807727D-04	6.343683250D-08					
-7.068589480D-12	3.335435980D-16		5.848134850D+03	-2.350925275D+01					
Ca(a) Alpha. Ref-Elm. Alcock,1993.									
2 srd 93 CA	1.00	0.00	0.00	0.00	0.00	1	40.0780000	0.000	
200.000	298.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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
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	40.0780000	0.000	
716.000	1115.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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	40.0780000	0.000	
1115.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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					
CaBr2(cr) Rhombic Gurvich,1996a pt1 p473 pt2 p368.									
1 tpis96 CA	1.00BR	2.00	0.00	0.00	0.00	1	199.8860000	-683800.000	
298.150	1015.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.826384237D+04	0.000000000D+00	8.872561342D+00	1.586623866D-03	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-8.505243950D+04	-3.554898721D+01					
CaBr2(L) Liquid Gurvich,1996a pt1 p473 pt2 p368.									
1 tpis96 CA	1.00BR	2.00	0.00	0.00	0.00	2	199.8860000	-683800.000	
1015.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	1.202716696D+01	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-8.390932270D+04	-5.231487518D+01					
CaCO3(cr) Hexagonal Gurvich,1996a pt1 p483 pt2 p376.									
2 tpis96 CA	1.00C	1.000	3.00	0.00	0.00	1	100.0869000	-1206600.000	
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.329862425D+07	2.500517168D+05	-1.907177167D+03	7.616666270D+00	-1.655870860D-02					
1.879382277D-05	8.720713270D-09		-1.271058215D+06	9.957497560D+03					
500.000	1603.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.58355736D+05	0.000000000D+00	1.197256363D+01	3.263812299D-03	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-1.497009803D+05	-5.961133653D+01					
CaCO3(L) Liquid Gurvich,1996a pt1 p483 pt2 p376.									
1 tpis96 CA	1.00C	1.000	3.00	0.00	0.00	3	100.0869000	-1206600.000	
1603.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
0.000000000D+00	0.000000000D+00	1.924346714D+01	0.000000000D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-1.526719277D+05	-1.052847193D+02					
CaCL2(cr) Rhombic. Gurvich,1996a pt1 p467 pt2 p365.									
2 tpis96 CA	1.00CL	2.00	0.00	0.00	0.00	1	110.9840000	-795800.000	
100.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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
-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. Gurvich,1996a pt1 p467 pt2 p365.									
1 tpis96 CA	1.00CL	2.00	0.00	0.00	0.00	2	110.9840000	-795800.000	
1048.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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					

## Appendix D (continued)

CaF2(a) CrII,cubic.Gurvich,1996a pt1 p461 pt2 p361.  
 3 tps96 CA 1.00F 2.00 0.00 0.00 0.00 1 78.0748064 -1228000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11640.000  
 -9.875281260D+05 1.337426670D+04-6.261903110D+01 1.617894422D-01-1.271795719D-04  
 0.000000000D+00 0.000000000D+00 -2.146045473D+05 3.617287210D+02  
 500.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11640.000  
 -6.961842180D+06 4.692065010D+04-1.157708151D+02 1.655025287D-01-1.108459197D-04  
 3.213053720D-08 0.000000000D+00 -4.101016540D+05 7.419533450D+02  
 1000.000 1424.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11640.000  
 1.438558077D+09 7.852955040D+05-1.342916213D+04 2.192783112D+01-1.383442475D-02  
 3.122877330D-06 0.000000000D+00 2.168972069D+06 7.823794920D+04

CaF2(b) CrI,cubic.Gurvich,1996a pt1 p461 pt2 p361.  
 1 tps96 CA 1.00F 2.00 0.00 0.00 0.00 2 78.0748064 -1228000.000  
 1424.000 1691.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11640.000  
 1.535768139D+08 0.000000000D+00-1.699774473D+02 7.733123360D-02 3.585714680D-07  
 0.000000000D+00 0.000000000D+00 1.356828739D+05 1.185723820D+03

CaF2(L) Liquid.Gurvich,1996a pt1 p461 pt2 p361.  
 1 tps96 CA 1.00F 2.00 0.00 0.00 0.00 3 78.0748064 -1228000.000  
 1691.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11640.000  
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.479539740D+05-5.967665213D+01

CaH2(a) CrII,rhombic.Gurvich,1996a pt1 p449 pt2 p354.  
 1 tps96 CA 1.00H 2.00 0.00 0.00 0.00 1 42.0938800 -177000.000  
 298.150 1053.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6770.474  
 0.000000000D+00 0.000000000D+00 3.599731073D+00 4.465566822D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.255982511D+04-1.686197756D+01

CaH2(b) CrI,cubic.Gurvich,1996a pt1 p449 pt2 p354.  
 1 tps96 CA 1.00H 2.00 0.00 0.00 0.00 2 42.0938800 -177000.000  
 1053.000 1273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6770.474  
 0.000000000D+00 0.000000000D+00 8.298745206D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.422633646D+04-4.409678633D+01

CaH2(L) Liquid.Gurvich,1996a pt1 p449 pt2 p354.  
 1 tps96 CA 1.00H 2.00 0.00 0.00 0.00 3 42.0938800 -177000.000  
 1273.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6770.474  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.249899474D+04-4.717727797D+01

CaI2(cr) Hexagonal.Gurvich,1996a pt1 p476 pt2 p371.  
 2 tps96 CA 1.00I 2.00 0.00 0.00 0.00 1 293.8869400 -536400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17970.499  
 -1.811328452D+06 3.127451814D+04-2.136599007D+02 8.328705880D-01-1.721725832D-03  
 1.878967812D-06-8.440013400D-10 -2.101977983D+05 1.142802698D+03  
 500.000 1056.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17970.499  
 -6.638996165D+03 0.000000000D+00 8.652825001D+00 2.284560365D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.721736780D+04-3.254333551D+01

CaI2(L) Liquid.Gurvich,1996a pt1 p476 pt2 p371.  
 1 tps96 CA 1.00I 2.00 0.00 0.00 0.00 3 293.8869400 -536400.000  
 1056.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17970.499  
 0.000000000D+00 0.000000000D+00 1.238798197D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.485425310D+04-5.137218163D+01

CaO(cr) Cubic.Gurvich,1996a pt1 p442 pt2 p348.  
 2 tps96 CA 1.00O 1.00 0.00 0.00 0.00 1 56.0774000 -634920.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6750.499  
 -4.775526940D+06 9.037711420D+04-6.944320810D+02 2.802477174D+00-6.129403220D-03  
 6.982167800D-06-3.247543840D-09 -4.829411430D+05 3.619046320D+03  
 500.000 3172.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6750.499  
 -1.459376440D+05 0.000000000D+00 7.174205094D+00-1.959947129D-03 1.291116374D-06  
 -2.077091735D-10 0.000000000D+00 -7.891525080D+04-3.658562837D+01

CaO(L) Liquid.Gurvich,1996a pt1 p442 pt2 p348.  
 1 tps96 CA 1.00O 1.00 0.00 0.00 0.00 3 56.0774000 -634920.000  
 3172.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6750.499  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.991857230D+04-5.908720013D+01

Ca(OH)2(cr) Hexagonal.Gurvich,1996a pt1 p454 pt2 p357.  
 2 tps96 CA 1.00O 2.00H 2.00 0.00 0.00 1 74.0926800 -985900.000  
 100.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14160.490  
 -2.058838935D+05 6.172554490D+03-7.499750990D+01 5.012182400D-01-1.423348682D-03  
 1.994984415D-06-1.095038067D-09 -1.452026205D+05 3.552445040D+02  
 500.000 1023.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14160.490  
 -1.245413139D+05 0.000000000D+00 1.073593032D+01 3.982435525D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.223707243D+05-5.302395390D+01

## Appendix D (continued)

Ca(OH)2(L) Liquid Gurvich,1996a pt1 p454 pt2 p357.  
 1 tpis96 CA 1.000 2.00H 2.00 0.00 0.00 3 74.0926800 -985900.000  
 1023.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14160.490  
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.245191822D+05-9.860760364D+01

CaS(cr) Cubic Gurvich,1996a pt1 p478 pt2 p373.  
 2 tpis96 CA 1.00S 1.00 0.00 0.00 0.00 1 72.1430000 -475000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9010.499  
 4.758681130D+06-8.840702110D+04 6.675047510D+02-2.576855161D+00 5.527281760D-03  
 -6.202901900D-06 2.852128154D-09 3.401344700D+05-3.494344760D+03  
 500.000 2800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9010.499  
 -1.428827435D+04 0.000000000D+00 5.567375588D+00 1.006673875D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.888163400D+04-2.530572359D+01

CaS(L) Liquid Gurvich,1996a pt1 p478 pt2 p373.  
 1 tpis96 CA 1.00S 1.00 0.00 0.00 0.00 3 72.1430000 -475000.000  
 2800.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9010.499  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.348566620D+04-3.924995523D+01

CaSO4(II) Rhombic Gurvich,1996a pt1 p481 pt2 p375.  
 2 tpis96 CA 1.00S 1.000 4.00 0.00 0.00 1 136.1406000 -1434000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17200.499  
 -1.361977472D+07 2.584929291D+05-1.984800641D+03 7.969448170D+00-1.736805219D-02  
 1.974370111D-05-9.168768090D-09 -1.334631522D+06 1.035139350D+04  
 500.000 1473.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17200.499  
 -2.983940124D+05 0.000000000D+00 1.359671225D+01 5.857230312D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.777846313D+05-6.802481458D+01

CaSO4(I) Cubic Gurvich,1996a pt1 p481 pt2 p375.  
 1 tpis96 CA 1.00S 1.000 4.00 0.00 0.00 3 136.1406000 -1434000.000  
 1473.000 1733.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17200.499  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.798298668D+05-1.045004358D+02

CaSO4(L) Liquid Gurvich,1996a pt1 p481 pt2 p375.  
 1 tpis96 CA 1.00S 1.000 4.00 0.00 0.00 4 136.1406000 -1434000.000  
 1733.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17200.499  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.764622601D+05-1.025572120D+02

Cd(cr) Crystal. Ref-Elm. Cox,1989 p223.  
 1 coda89 CD 1.00 0.00 0.00 0.00 0.00 1 112.4110000 0.000  
 100.000 594.2587 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6247.000  
 1.375273221D+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 2 112.4110000 0.000  
 594.258 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6247.000  
 0.000000000D+00 0.000000000D+00 3.596122922D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.220394750D+02-1.323298164D+01

Co(a) Alpha. Ref-Elm. Chase,1998 pp943-6.  
 2 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 1 58.9332000 0.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4771.000  
 -8.651834510D+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 pp943-6.  
 2 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 2 58.9332000 0.000  
 700.100 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4771.000  
 0.000000000D+00 0.000000000D+00 2.125113886D+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

Co(b) Beta. Ref-Elm. Above Lambda trans. Chase,1998 pp943-6.  
 2 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 3 58.9332000 0.000  
 1394.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4771.000  
 0.000000000D+00 0.000000000D+00 3.070872109D+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

## Appendix D (continued)

Co(L) Liquid. Ref-Elm. Chase,1998 pp943-6.  
 1 j 9/67 CO 1.00 0.00 0.00 0.00 0.00 4 58.9332000 0.000  
 1768.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4771.000  
 0.000000000D+00 0.000000000D+00 4.871122892D+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 pp959-62.  
 1 j 6/73 CR 1.00 0.00 0.00 0.00 0.00 1 51.9961000 0.000  
 200.000 311.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4057.000  
 8.051084050D+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 pp959-62.  
 2 j 6/73 CR 1.00 0.00 0.00 0.00 0.00 2 51.9961000 0.000  
 311.500 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4057.000  
 -2.534425357D+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 pp959-62.  
 1 j 6/73 CR 1.00 0.00 0.00 0.00 0.00 3 51.9961000 0.000  
 2130.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4057.000  
 0.000000000D+00 0.000000000D+00 4.730284767D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 5.755633080D+02-2.453179007D+01  
 CrN(cr) Chase,1998 p966.  
 3 j12/73 CR 1.00N 1.00 0.00 0.00 0.00 1 66.0028000 -117152.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7705.000  
 0.000000000D+00 0.000000000D+00-1.314063090D+00 2.565693051D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.483864491D+04 4.372952650D+00  
 298.150 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7705.000  
 1.223200207D+06 0.000000000D+00-2.407090178D+01 5.583146740D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.292218790D+03 1.319158541D+02  
 400.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7705.000  
 -2.661907798D+05 1.615547039D+03 1.892576742D+00 4.987173370D-03-2.514705667D-06  
 7.617792270D-10-9.124276740D-14 -2.496407842D+04-3.735659490D+00  
 Cr2N(cr) JPCRD 1998 Mono.9 p971.  
 3 j12/73 CR 2.00N 1.00 0.00 0.00 0.00 1 117.9989000 -125520.000  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 5.676714650D+06-6.561919460D+04 2.971622148D+02-6.132148300D-01 6.373067250D-04  
 -2.569754132D-07 0.000000000D+00 3.113488256D+05-1.716694497D+03  
 700.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 8.246680410D+05-1.965549089D+03 5.659967790D+00 1.366241998D-02-1.241835551D-05  
 6.313550760D-09-1.192405400D-12 -3.594772610D+03-3.071970867D+01  
 1500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 4.325258320D+09-1.355254539D+07 1.757503878D+04-1.205560629D+01 4.623646210D-03  
 -9.389890050D-07 7.891119490D-11 8.506076540D+07-1.227417790D+05  
 Cr2O3(I') Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.  
 1 tpis82 CR 2.000 3.00 0.00 0.00 0.00 1 151.9904000 -1140600.000  
 200.000 306.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15300.000  
 -2.112979833D+06 0.000000000D+00 2.207431906D+02-1.164973854D+00 1.853971249D-03  
 0.000000000D+00 0.000000000D+00 -1.746831159D+05-9.949025210D+02  
 Cr2O3(I) Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.  
 1 tpis82 CR 2.000 3.00 0.00 0.00 0.00 2 151.9904000 -1140600.000  
 306.000 310.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15300.000  
 0.000000000D+00 0.000000000D+00 6.705915562D+03-4.303760534D+01 6.919229155D-02  
 0.000000000D+00 0.000000000D+00 -8.349875160D+05-2.844167579D+04  
 Cr2O3(I) Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.  
 1 tpis82 CR 2.000 3.00 0.00 0.00 0.00 3 151.9904000 -1140600.000  
 310.000 335.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15300.000  
 0.000000000D+00 0.000000000D+00 2.443570337D+02-1.399445548D+00 2.113509996D-03  
 0.000000000D+00 0.000000000D+00 -1.665032895D+05-1.059172219D+03  
 Cr2O3(I) Hexagonal. Gurvich,1982 pt1 p18 pt2 p22.  
 1 tpis82 CR 2.000 3.00 0.00 0.00 0.00 4 151.9904000 -1140600.000  
 335.000 2705.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15300.000  
 -3.415474875D+05 0.000000000D+00 1.616932327D+01-1.517828471D-03 1.014852348D-06  
 0.000000000D+00 0.000000000D+00 -1.430478214D+05-8.374919535D+01  
 Cr2O3(L) Liquid. Gurvich,1982 pt1 p18 pt2 p22.  
 1 tpis82 CR 2.000 3.00 0.00 0.00 0.00 5 151.9904000 -1140600.000  
 2705.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15300.000  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.383139935D+05-1.123603099D+02

## Appendix D (continued)

Cs(cr) Crystal. Ref-Elm. Cox,1989 p263.

1 coda89 CS	1.00	0.00	0.00	0.00	0.00	1	132.9054500	0.000
100.000	301.5907	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
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	132.9054500	0.000
301.590	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-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
-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

CsBO2(cr) Cubic. Gurvich,1982 pt1 p504 pt2 p525.

2 tpis82 CS	1.00B	1.000	2.00	0.00	0.00	1	175.7152500	-962000.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.241529552D+07	-2.256720327D+05	1.662515290D+03	-6.320716230D+00	1.337407484D-02	-1.484168930D-05	6.761667750D-09	9.049643320D+05	-8.739017110D+03
500.000	1005.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.344267330D+05	0.000000000D+00	1.014162565D+01	3.564309650D-03	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.193344436D+05	-4.705131010D+01

CsBO2(L) Liquid. Gurvich,1982 pt1 p504 pt2 p525.

1 tpis82 CS	1.00B	1.000	2.00	0.00	0.00	2	175.7152500	-962000.000
1005.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.743939210D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.214875849D+05	-9.061903610D+01

CsBr(cr) Cubic. Gurvich,1982 pt1 p488 pt2 p511.

2 tpis82 CS	1.00BR	1.00	0.00	0.00	0.00	1	212.8094500	-405600.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.214717410D+05	-1.533809444D+04	1.213999610D+02	-4.502622350D-01	9.722874060D-04	-1.094185412D-06	5.042592550D-10	1.851486523D+04	-6.252270680D+02
500.000	910.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	5.882254010D+00	1.622332026D-03	0.000000000D+00	0.000000000D+00	0.000000000D+00	-5.060809300D+04	-2.041491096D+01

CsBr(L) Liquid. Gurvich,1982 pt1 p488 pt2 p511.

1 tpis82 CS	1.00BR	1.00	0.00	0.00	0.00	2	212.8094500	-405600.000
910.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	9.020375224D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-4.995364530D+04	-3.720087044D+01

CsCL(a) Cubic. Gurvich,1982 pt1 p485 pt2 p508.

2 tpis82 CS	1.00CL	1.00	0.00	0.00	0.00	1	168.3584500	-442310.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.703772998D+06	3.247452440D+04	-2.455466631D+02	1.009178034D+00	-2.207551915D-03	2.517334138D-06	-1.172381667D-09	-2.005014179D+05	1.287839193D+03
500.000	743.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.937950690D+04	0.000000000D+00	6.626999920D+00	4.235262420D-04	0.000000000D+00	0.000000000D+00	0.000000000D+00	-5.532407590D+04	-2.593783387D+01

CsCL(b) Cubic. Gurvich,1982 pt1 p485 pt2 p508.

1 tpis82 CS	1.00CL	1.00	0.00	0.00	0.00	2	168.3584500	-442310.000
743.000	919.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	7.841712861D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-5.570430740D+04	-3.314329722D+01

CsCL(L) Liquid. Gurvich,1982 pt1 p485 pt2 p508.

1 tpis82 CS	1.00CL	1.00	0.00	0.00	0.00	3	168.3584500	-442310.000
919.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	8.839967719D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-5.417056700D+04	-3.728749769D+01

CsF(cr) Cubic. Gurvich,1982 pt1 p481 pt2 p505.

2 tpis82 CS	1.00F	1.00	0.00	0.00	0.00	1	151.9038532	-557100.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.453746682D+06	4.440981600D+04	-3.216355300D+02	1.258524529D+00	-2.661147803D-03	2.959315715D-06	-1.350383298D-09	-2.700040022D+05	1.698453355D+03
500.000	976.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	5.088206230D+00	3.543462080D-03	0.000000000D+00	0.000000000D+00	0.000000000D+00	-6.867788740D+04	-1.886662026D+01

CsF(L) Liquid. Gurvich,1982 pt1 p481 pt2 p505.

1 tpis82 CS	1.00F	1.00	0.00	0.00	0.00	2	151.9038532	-557100.000
976.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	8.659560215D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-6.786592520D+04	-3.731740982D+01

## Appendix D (continued)

CsH(cr) Cubic. Gurvich,1982 pt1 p476 pt2 p500.  
 1 tpis82 CS 1.00H 1.00 0.00 0.00 0.00 1 133.9133900 -54040.000  
 298.150 801.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10500.000  
 -5.041788392D+04 0.000000000D+00 4.142517118D+00 4.385946977D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.098615840D+03 -1.641381626D+01

CsH(L) Liquid. Gurvich,1982 pt1 p476 pt2 p500.  
 1 tpis82 CS 1.00H 1.00 0.00 0.00 0.00 2 133.9133900 -54040.000  
 801.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10500.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.901332940D+03 -2.794351109D+01

CsI(cr) Cubic. Gurvich,1982 pt1 p492 pt2 p514.  
 2 tpis82 CS 1.00I 1.00 0.00 0.00 0.00 1 259.8099200 -348100.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13470.000  
 1.754014150D+06 -3.232916500D+04 2.467159187D+02 -9.287377130D-01 1.973235969D-03  
 -2.193580686D-06 1.003390730D-09 1.023639971D+05 -1.282961001D+03  
 500.000 905.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13470.000  
 -1.690343843D+04 0.000000000D+00 7.346625000D+00 -4.804073480D-03 6.604565720D-06  
 0.000000000D+00 0.000000000D+00 -4.395851780D+04 -2.611726446D+01

CsI(L) Liquid. Gurvich,1982 pt1 p492 pt2 p514.  
 1 tpis82 CS 1.00I 1.00 0.00 0.00 0.00 2 259.8099200 -348100.000  
 905.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13470.000  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.226975350D+04 -3.246075054D+01

CsNO2(I) Cubic. Gurvich,1982 pt1 p498 pt2 p519.  
 1 tpis82 CS 1.00N 1.000 2.00 0.00 0.00 1 178.9109500 -379900.000  
 298.150 679.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23420.000  
 0.000000000D+00 0.000000000D+00 1.151300558D+01 -3.537430348D-03 5.931437932D-06  
 0.000000000D+00 0.000000000D+00 -4.901898420D+04 -4.387814029D+01

CsNO2(L) Liquid. Gurvich,1982 pt1 p498 pt2 p519.  
 1 tpis82 CS 1.00N 1.000 2.00 0.00 0.00 2 178.9109500 -379900.000  
 679.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23420.000  
 0.000000000D+00 0.000000000D+00 1.274879698D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.874363630D+04 -5.104014160D+01

CsNO3(a) Hexagonal. Gurvich,1982 pt1 p500 pt2 p521.  
 1 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 1 194.9103500 -505000.000  
 200.000 427.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20050.000  
 -3.246405120D+06 5.377946540D+04 -3.399293910D+02 1.103526542D+00 -1.665374892D-03  
 1.005891643D-06 0.000000000D+00 -3.130119262D+05 1.853516509D+03

CsNO3(b) Cubic. Gurvich,1982 pt1 p500 pt2 p521.  
 1 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 2 194.9103500 -505000.000  
 427.000 682.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20050.000  
 -8.675315803D+05 0.000000000D+00 2.211459244D+01 -4.596061584D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.970758310D+04 -1.102656798D+02

CsNO3(L) Cubic. Gurvich,1982 pt1 p500 pt2 p521.  
 1 tpis82 CS 1.00N 1.000 3.00 0.00 0.00 3 194.9103500 -505000.000  
 682.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20050.000  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.506630270D+04 -8.345202339D+01

CsOH(b) Beta. Gurvich,1997.  
 2 g 8/97 CS 1.000 1.00H 1.00 0.00 0.00 1 149.9127900 -416200.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.000  
 -1.070491244D+06 2.726790967D+04 -2.447999195D+02 9.717566950D-01 -1.304183626D-03  
 0.000000000D+00 0.000000000D+00 -1.676915176D+05 1.260979156D+03  
 298.150 498.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.000  
 2.988510447D+05 0.000000000D+00 -5.599488124D+00 4.758933479D-02 -3.982976748D-05  
 0.000000000D+00 0.000000000D+00 -4.914854260D+04 3.370083195D+01

CsOH(c) Gamma. Gurvich,1997.  
 1 g 8/97 CS 1.000 1.00H 1.00 0.00 0.00 3 149.9127900 -416200.000  
 498.200 615.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.000  
 0.000000000D+00 0.000000000D+00 8.743750383D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.198053970D+04 -3.591737929D+01

CsOH(L) Liquid. Gurvich,1997.  
 1 g 8/97 CS 1.000 1.00H 1.00 0.00 0.00 4 149.9127900 -416200.000  
 615.500 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14103.000  
 0.000000000D+00 0.000000000D+00 1.022309192D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.195536080D+04 -4.389810453D+01

CsO2(a) Tetragonal. Gurvich,1982 pt1 p472 pt2 p494.  
 1 tpis82 CS 1.00O 2.00 0.00 0.00 0.00 1 164.9042500 -286100.000  
 298.150 403.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18000.000  
 0.000000000D+00 0.000000000D+00 6.423469330D+00 1.032375931D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.678373920D+04 -2.259778952D+01



## Appendix D (continued)

CsO2(c) Cubic. Gurvich,1982 pt1 p472 pt2 p494.  
 1 tpis82 CS 1.000 2.00 0.00 0.00 0.00 0.00 2 164.9042500 -286100.000  
 403.000 723.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18000.000  
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.762205990D+04-4.339551574D+01

CsO2(L) Liquid. Gurvich,1982 pt1 p472 pt2 p494.  
 1 tpis82 CS 1.000 2.00 0.00 0.00 0.00 0.00 3 164.9042500 -286100.000  
 723.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18000.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.645253810D+04-4.983623140D+01

Cs2CO3(cr) Gurvich,1982 pt1 p502 pt2 p523.  
 2 tpis82 CS 2.00C 1.000 3.00 0.00 0.00 0.00 1 325.8198000 -1134900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 25727.000  
 -2.861109977D+06 6.041289230D+04-5.002404530D+02 2.198717904D+00-5.002265900D-03  
 5.885981300D-06-2.807201102D-09 -4.049923380D+05 2.581625553D+03  
 500.000 1066.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 25727.000  
 -2.194678436D+05 0.000000000D+00 1.478581229D+01 8.646042770D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.420250493D+05-6.346394980D+01

Cs2CO3(L) Liquid. Gurvich,1982 pt1 502 pt2 p523.  
 1 tpis82 CS 2.00C 1.000 3.00 0.00 0.00 0.00 2 325.8198000 -1134900.000  
 1066.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 25727.000  
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.436995486D+05-1.194626528D+02

Cs2O(cr) Hexagonal. Gurvich,1982 pt1 p472 pt2 p495.  
 2 tpis82 CS 2.000 1.00 0.00 0.00 0.00 0.00 1 281.8103000 -346400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17680.000  
 -5.627068090D+05 9.379197410D+03-5.661406600D+01 2.388479040D-01-4.761089540D-04  
 5.101511920D-07-2.256975084D-10 -8.742010290D+04 3.144128417D+02  
 500.000 768.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17680.000  
 0.000000000D+00 0.000000000D+00 7.940814720D+00 4.024410190D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.420852680D+04-2.877552024D+01

Cs2O(L) Liquid. Gurvich,1982 pt1 p472 pt2 p495.  
 1 tpis82 CS 2.000 1.00 0.00 0.00 0.00 0.00 2 281.8103000 -346400.000  
 768.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17680.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.375456510D+04-4.970156357D+01

Cs2O2(cr) Rhombic Gurvich,1982 pt1 p475 pt2 p498.  
 1 tpis82 CS 2.000 2.00 0.00 0.00 0.00 0.00 1 297.8097000 -440000.000  
 298.150 867.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21300.000  
 0.000000000D+00 0.000000000D+00 1.003895599D+01 4.651506824D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.611939360D+04-3.693586892D+01

Cs2O2(L) Liquid. Gurvich,1982 pt1 p475 pt2 p498.  
 1 tpis82 CS 2.000 2.00 0.00 0.00 0.00 0.00 2 297.8097000 -440000.000  
 867.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 21300.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.699432080D+04-7.096530706D+01

Cs2SO4(a) Rhombohedral. Gurvich,1982 pt1 p496 pt2 p517.  
 2 tpis82 CS 2.00S 1.000 4.00 0.00 0.00 0.00 1 361.8735000 -1442900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27740.000  
 -9.607719290D+06 1.823999086D+05-1.398882747D+03 5.671901780D+00-1.240281336D-02  
 1.414114808D-05-6.571017390D-09 -9.952928170D+05 7.301725680D+03  
 500.000 920.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27740.000  
 -2.673923999D+05 0.000000000D+00 1.731761674D+01 9.163180750D-03-1.678705593D-05  
 2.444634119D-08 0.000000000D+00 -1.799058942D+05-7.688396220D+01

Cs2SO4(b) Gurvich,1982 pt1 p496 pt2 p517.  
 1 tpis82 CS 2.00S 1.000 4.00 0.00 0.00 0.00 2 361.8735000 -1442900.000  
 920.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27740.000  
 0.000000000D+00 0.000000000D+00-2.345297558D+01 5.324523033D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.607408251D+05 1.601933430D+02

Cs2SO4(c) Hexagonal. Gurvich,1982 pt1 p496 pt2 p517.  
 1 tpis82 CS 2.00S 1.000 4.00 0.00 0.00 0.00 3 361.8735000 -1442900.000  
 1000.000 1288.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27740.000  
 0.000000000D+00 0.000000000D+00 1.021611616D+01 1.412157782D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.748480906D+05-3.326085070D+01

Cs2SO4(L) Liquid. Gurvich,1982 pt1 p496 pt2 p517.  
 1 tpis82 CS 2.00S 1.000 4.00 0.00 0.00 0.00 4 361.8735000 -1442900.000  
 1288.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 27740.000  
 0.000000000D+00 0.000000000D+00 2.489623562D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.778210954D+05-1.169167420D+02

## Appendix D (continued)

Cu(cr) Cubic. Ref-Elm.Cox,1989 p226.  
 1 coda89 CU 1.00 0.00 0.00 0.00 0.00 1 63.5460000 0.000  
 200.000 1358.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5004.000  
 -2.455775109D+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 63.5460000 0.000  
 1358.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5004.000  
 0.000000000D+00 0.000000000D+00 3.944910764D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.111013775D+02-1.836065775D+01

CuBr(a) Alpha. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 1 143.4500000 -105604.160  
 298.150 657.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 9.282973940D+07-1.403844530D+06 8.783223470D+03-2.905323712D+01 5.373393350D-02  
 -5.266133060D-05 2.137926033D-08 6.589039380D+06-4.752115490D+04

CuBr(b) Beta. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 2 143.4500000 -105604.160  
 657.000 741.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 2.030134717D+04 0.000000000D+00 8.680899310D+00 1.192698187D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.494845171D+04-3.784920540D+01

CuBr(c) Gamma. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 3 143.4500000 -105604.160  
 741.000 759.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 6.996549990D+00-2.480878428D-06 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.343768009D+04-2.630094995D+01

CuBr(L) Liquid. Pankratz,1984 p177.  
 1 g10/00 CU 1.00BR 1.00 0.00 0.00 0.00 4 143.4500000 -105604.160  
 759.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 5.249558100D+06-2.757081290D+04 7.103036660D+01-7.368389880D-02 4.263508020D-05  
 -1.219118967D-08 1.489531692D-12 1.442863364D+05-4.366365590D+02

CuBr2(cr) Crystal. Pankratz,1984 p181.  
 1 g10/00 CU 1.00BR 2.00 0.00 0.00 0.00 1 223.3540000 -138490.400  
 298.150 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -2.314796663D+04 0.000000000D+00 9.183704151D+00 6.239886656D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.949996594D+04-3.714221219D+01

CuCL(a) Alpha. Pankratz,1984 p182.  
 1 g10/00 CU 1.00CL 1.00 0.00 0.00 0.00 1 98.9990000 -155644.800  
 298.150 685.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -3.658126050D+07 4.622460750D+05-2.297616527D+03 5.656465110D+00-6.837763380D-03  
 3.261042890D-06 0.000000000D+00 -2.287516266D+06 1.303469843D+04

CuCL(b) Beta. Pankratz,1984 p182.  
 1 g10/00 CU 1.00CL 1.00 0.00 0.00 0.00 2 98.9990000 -155644.800  
 685.000 696.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 9.573589740D+00-1.820889604D-05 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.177033413D+04-4.503412690D+01

CuCL(L) Liquid. Pankratz,1984 p182.  
 1 g10/00 CU 1.00CL 1.00 0.00 0.00 0.00 3 98.9990000 -155644.800  
 696.000 1700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 2.136369978D+07-1.123842012D+05 2.576303311D+02-2.967521373D-01 1.937139129D-04  
 -6.602332990D-08 9.216872010D-12 6.263960470D+05-1.640361694D+03

CuCL2(cr) Crystal. Pankratz,1984 p185.  
 1 g10/00 CU 1.00CL 2.00 0.00 0.00 0.00 1 134.4520000 -217986.400  
 298.150 675.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -2.119456576D+04-7.996037250D+02 1.293400534D+01-6.531311580D-03 7.387791880D-06  
 -2.975231314D-09 0.000000000D+00 -2.535822405D+04-6.185052500D+01

CuCL2(L) Liquid. Pankratz,1984 p185.  
 1 g10/00 CU 1.00CL 2.00 0.00 0.00 0.00 2 134.4520000 -217986.400  
 675.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 9.913368316D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.929700009D+04-4.386870689D+01

CuF(cr) Crystal. Pankratz,1984 p186.  
 1 g10/00 CU 1.00F 1.00 0.00 0.00 0.00 1 82.5444032 -209200.000  
 298.150 1300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 8.970191630D+04-8.507461080D+02 7.497889560D+00 2.741560003D-03-2.987072214D-06  
 1.372974641D-09-2.449154828D-13 -2.234632002D+04-3.796523780D+01

CuF2(cr) Crystal. Pankratz,1984 p188.  
 1 g10/00 CU 1.00F 2.00 0.00 0.00 0.00 1 101.5428064 -539819.680  
 298.150 1109.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 2.173703718D+04-4.937180300D+02 7.140314880D+00 9.517087050D-03-7.459164380D-06  
 1.904472482D-09 4.473847180D-13 -6.452906470D+04-3.535501070D+01

## Appendix D (continued)

CuF2(L) Liquid. Pankratz,1984 p188.  
 1 g10/00 CU 1.00F 2.00 0.00 0.00 0.00 2 101.5428064 -539819.680  
 1109.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 1.207719998D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.351133500D+04-5.654007188D+01

CuI(a) King,1973. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 2 190.4504700 -67780.800  
 200.000 642.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12179.624  
 3.341893600D+07-6.258598240D+05 4.752824990D+03-1.866377479D+01 4.013741700D-02  
 -4.477073620D-05 2.026229192D-08 2.806623546D+06-2.484310642D+04

CuI(b) Beta. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 2 190.4504700 -67780.800  
 642.000 680.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12179.624  
 0.000000000D+00 0.000000000D+00 1.665647164D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.582086031D+04-8.975455543D+01

CuI(c) Gamma. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 3 190.4504700 -67780.800  
 680.000 868.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12179.624  
 0.000000000D+00 0.000000000D+00 8.252753319D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.787795700D+03-3.447628919D+01

CuI(L) Liquid. Pankratz,1984 p190.  
 1 g11/00 CU 1.00I 1.00 0.00 0.00 0.00 4 190.4504700 -67780.800  
 868.000 1600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12179.624  
 -1.011252768D+08 4.982205420D+05-1.002812164D+03 1.087833779D+00-6.564648130D-04  
 2.096109501D-07-2.761239948D-11 -2.912510925D+06 6.575842050D+03

CuO(cr) Crystal. King,1973 p56.  
 2 g11/00 CU 1.00O 1.00 0.00 0.00 0.00 1 79.5454000 -155644.800  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7100.248  
 -4.516917320D+05 5.470078090D+03-2.199474390D+01 5.929815860D-02-4.346152590D-05  
 0.000000000D+00 0.000000000D+00 -4.709485370D+04 1.305030297D+02  
 500.000 1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7100.248  
 1.200465628D+06-7.265787600D+03 2.078520457D+01-1.455522591D-02 1.267438982D-05  
 -1.010207859D-08 3.818025500D-12 2.099455971D+04-1.272540351D+02

Cu(OH)2(cr) Crystal. King,1973 p62.  
 1 g10/00 CU 1.00O 2.00H 2.00 0.00 0.00 1 97.5606800 -443085.600  
 298.150 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -2.719377798D+05 2.064524617D+03 2.639692948D+00 1.680803576D-02-1.185312108D-05  
 4.128854220D-09-5.731701790D-13 -6.740281360D+04-3.697949500D+00

CuS(cr) Crystal. Pankratz,1987 p99.  
 1 g10/00 CU 1.00S 1.00 0.00 0.00 0.00 1 95.6110000 -55647.200  
 298.150 717.8247 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -2.883682516D+06 3.709375520D+04-1.908896435D+02 5.441914820D-01-8.255987560D-04  
 6.585650750D-07-2.151268669D-10 -1.888895944D+05 1.072934856D+03

CuSO4(cr) Crystal. King,1973 p68.  
 2 g10/00 CU 1.00S 1.00O 4.00 0.00 0.00 1 159.6086000 -768600.800  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16869.888  
 -6.059594400D+06 1.149925970D+05-8.865821710D+02 3.621436210D+00-7.953212370D-03  
 9.136099910D-06 4.293593660D-09 -6.103352510D+05 4.617693800D+03  
 500.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16869.888  
 4.517267510D+06-3.693547470D+04 1.240090231D+02-1.574474634D-01 1.231374136D-04  
 -4.209750670D-08 3.791447690D-12 1.020928632D+05-7.502604750D+02

Cu2O(cr) Crystal. King,1973 p60.  
 2 g10/00 CU 2.00O 1.00 0.00 0.00 0.00 1 143.0914000 -170707.200  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12598.024  
 6.943093940D+05-1.107206812D+04 7.007600820D+01-1.693010736D-01 2.296941394D-04  
 -1.193708373D-07 0.000000000D+00 2.971995795D+04-3.800603570D+02  
 600.000 1516.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12598.024  
 4.899293250D+06-3.226767710D+04 9.242913240D+01-1.133053506D-01 8.886458460D-05  
 -3.911779590D-08 8.170753140D-12 1.562364374D+05-5.668285450D+02

Cu2O(L) Liquid. King,1973 p60.  
 1 g10/00 CU 2.00O 1.00 0.00 0.00 0.00 2 143.0914000 -170707.200  
 1516.700 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12598.024  
 0.000000000D+00 0.000000000D+00 1.199819496D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.922442298D+04-5.674847630D+01

Cu2S(a) Alpha. Pankratz,1987 p101.  
 1 g10/00 CU 2.00S 1.00 0.00 0.00 0.00 1 159.1570000 -75730.400  
 298.150 376.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 1.219944245D+05 0.000000000D+00 2.442685885D+00 1.822933284D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.023757104D+04-4.696533160D+00

## Appendix D (continued)

Cu<sub>2</sub>S(b)                      Beta. Pankratz,1987 p101.  
 1 g10/00 CU   2.00S   1.00   0.00   0.00   0.00   2   159.1570000   -75730.400  
                  376.000   720.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      0.000  
 -1.211638496D+06 1.256233530D+04-3.683304810D+01 9.547244050D-02-9.864227170D-05  
 3.946755750D-08 0.000000000D+00                      -7.698051300D+04 2.352740334D+02

Cu<sub>2</sub>S(c)                      Gamma. Pankratz,1987 p101.  
 1 g10/00 CU   2.00S   1.00   0.00   0.00   0.00   3   159.1570000   -75730.400  
                  720.000   1400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      0.000  
 1.585983458D+07-9.420242290D+04 2.398981626D+02-2.943865388D-01 2.084368440D-04  
 -7.757369510D-08 1.184191791D-11                      5.203074640D+05-1.502163502D+03

Cu<sub>2</sub>S(L)                      Liquid. Pankratz,1987 p101.  
 1 g10/00 CU   2.00S   1.00   0.00   0.00   0.00   4   159.1570000   -75730.400  
                  1400.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      0.000  
 0.000000000D+00 0.000000000D+00 1.078393315D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -1.075259326D+04-4.551698813D+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   55.8450000   0.000  
                  200.000   500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      4507.000  
 1.350490931D+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 pp1221-5.  
 1 j 3/78 FE   1.00   0.00   0.00   0.00   0.00   2   55.8450000   0.000  
                  1042.000   1184.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      4507.000  
 2.481923052D+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 pp1221-5.  
 1 j 3/78 FE   1.00   0.00   0.00   0.00   0.00   3   55.8450000   0.000  
                  1184.000   1665.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      4507.000  
 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 pp1221-5.  
 1 j 3/78 FE   1.00   0.00   0.00   0.00   0.00   4   55.8450000   0.000  
                  1665.000   1809.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      4507.000  
 -3.450190030D+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 pp1221-5.  
 1 j 3/78 FE   1.00   0.00   0.00   0.00   0.00   5   55.8450000   0.000  
                  1809.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      4507.000  
 0.000000000D+00 0.000000000D+00 5.535383324D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -1.270608703D+03-2.948115042D+01

Fe(CO)5(L)                      Liquid. Chase,1998 p697.  
 1 j 3/78 FE   1.00C   5.00C   5.00   0.00   0.00   1   195.8955000   -766090.400  
                  253.100   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      52934.000  
 0.000000000D+00 0.000000000D+00 2.811771229D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -1.005222674D+05-1.196624513D+02

FeCL2(cr)                      Crystal. Chase,1998 pp819-21.  
 1 j12/70 FE   1.00CL   2.00   0.00   0.00   0.00   1   126.7510000   -341833.000  
                  200.000   950.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      16273.000  
 -3.757527240D+04 5.932070220D+00 8.822760280D+00 3.742344220D-03-4.622462850D-06  
 4.041497880D-09-1.447289303D-12                      -4.403595790D+04-3.721747350D+01

FeCL2(L)                      Liquid. Chase,1998 pp819-21.  
 1 j12/70 FE   1.00CL   2.00   0.00   0.00   0.00   2   126.7510000   -341833.000  
                  950.000   6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      16273.000  
 0.000000000D+00 0.000000000D+00 1.228851730D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -4.110842530D+04-5.319067642D+01

FeCL3(cr)                      Pankratz,1984 p228. Stuve,1980.  
 2 g12/00 FE   1.00CL   3.00   0.00   0.00   0.00   1   162.2040000   -399237.280  
                  200.000   298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      19440.538  
 -4.411357940D+06 9.339652130D+04-7.909985950D+02 3.467913380D+00-7.632263650D-03  
 7.316486370D-06-1.314023921D-09                      -4.596567330D+05 4.056239320D+03  
                  298.150   577.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0                      19440.538  
 -1.373170458D+05 1.246888186D+03 4.499842520D+00 1.632234838D-02-3.871665510D-06  
 0.000000000D+00 0.000000000D+00                      -5.761466240D+04-9.144353090D+00

## Appendix D (continued)

FeCl<sub>3</sub>(L) Pankratz,1984 p228. Stuve,1980.  
 1 g12/00 FE 1.00CL 3.00 0.00 0.00 0.00 2 162.2040000 -399237.280  
 577.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19440.538  
 0.000000000D+00 0.000000000D+00 1.610293331D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.849183540D+04-6.711333581D+01

Fe.9470(cr) Wustite. Pankratz,1983 p155.  
 1 g11/00 FE 0.950 1.00 0.00 0.00 0.00 1 69.0521500 -266269.760  
 298.150 1652.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -1.179193966D+04 1.388393372D+02 2.999841854D+00 1.274527210D-02-1.883886065D-05  
 1.274258345D-08-3.042206479D-12 -3.417350500D+04-1.284759120D+01

Fe.9470(L) Wustite Liquid. Pankratz,1983 p155.  
 1 g11/00 FE 0.950 1.00 0.00 0.00 0.00 2 69.0521500 -266269.760  
 1652.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 8.147077819D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.255080650D+04-3.995344357D+01

FeOCL(cr) Stuve,1980.  
 2 g12/00 FE 1.000 1.00CL 1.00 0.00 0.00 1 107.2974000 -410994.320  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12940.275  
 7.211593840D+08-1.800235674D+07 1.865368524D+05-1.026861036D+03 3.167682830D+00  
 -5.191522260D-08 3.531434870D-06 7.557107690D+07-9.148719350D+05  
 298.150 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12940.275  
 -2.937711808D+05 2.628264415D+03-4.552872200D+00 3.806463330D-02-5.536092880D-05  
 4.502460810D-08-1.258510270D-11 -6.531943100D+04 3.377057910D+01

Fe(OH)2(cr) Crystal. Chase,1998 p1229.  
 2 j 6/66 FE 1.000 2.00H 2.00 0.00 0.00 1 89.8596800 -574045.000  
 298.150 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 4.240926040D+05-5.246013500D+03 3.564078140D+01-5.777285350D-02 8.334162550D-05  
 -5.353404280D-08 1.183994084D-11 -4.642385900D+04-1.937387923D+02  
 800.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 8.260012740D+06-3.584848620D+04 6.631482130D+01-2.947893247D-02 4.572669670D-06  
 1.317544528D-09-2.977356578D-13 1.429652898D+05-4.364616280D+02

Fe(OH)3(cr) Crystal. Chase,1998 p1231.  
 1 j 6/66 FE 1.000 3.00H 3.00 0.00 0.00 1 106.8670200 -832616.000  
 298.150 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -7.418284690D+04 4.915361510D+01 6.351612700D+00 2.730299149D-02-2.006100982D-05  
 7.511526410D-09-1.262038044D-12 -1.036132609D+05-3.117351481D+01

FeS(a) Alpha. Pankratz,1987. Chase,1998 pp1241-3 9/77.  
 1 g11/00 FE 1.00S 1.00 0.00 0.00 0.00 1 87.9100000 -99621.040  
 200.000 411.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9414.000  
 6.562987140D+06-1.108882861D+05 7.200477640D+02-2.169002385D+00 3.009472055D-03  
 -1.385164934D-06 0.000000000D+00 4.996994470D+05-3.905129920D+03

FeS(b) Beta. Pankratz,1987. Chase,1998 pp1241-3 9/77.  
 1 g11/00 FE 1.00S 1.00 0.00 0.00 0.00 2 87.9100000 -99621.040  
 411.000 598.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9414.000  
 0.000000000D+00 0.000000000D+00 8.730809152D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.445777846D+04-4.227609187D+01

FeS(c) Gamma. Pankratz,1987. Chase,1998 pp1241-3 9/77.  
 1 g11/00 FE 1.00S 1.00 0.00 0.00 0.00 3 87.9100000 -99621.040  
 598.000 1465.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9414.000  
 -4.651400530D+05 2.845200913D+03 3.227601660D+00 1.639542844D-03-2.119596921D-06  
 2.366217205D-09-3.529138060D-13 -3.030024550D+04-3.662233560D+00

FeS(L) Liquid. Pankratz,1987. Chase,1998 pp1241-3 9/77.  
 1 g11/00 FE 1.00S 1.00 0.00 0.00 0.00 4 87.9100000 -99621.040  
 1465.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9414.000  
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.925935040D+03-3.215631501D+01

FeSO4(cr) Chase,1998 p1240.  
 2 j 6/66 FE 1.00S 1.000 4.00 0.00 0.00 1 151.9076000 -928848.000  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16769.472  
 -6.203392950D+05 8.502519150D+03-4.378024090D+01 1.731987422D-01-2.431424518D-04  
 1.792173046D-07-5.528922570D-11 -1.550636343D+05 2.467116078D+02  
 700.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16769.472  
 -7.679585180D+06 3.308117000D+04-4.678167570D+01 6.781223220D-02-3.741392130D-05  
 1.099952323D-08-1.320141816D-12 -3.134827612D+05 3.336437670D+02

## Appendix D (continued)

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FeS2(cr)          Pyrite. Chase,1998 p1246.
  2 j 9/77 FE  1.00S  2.00  0.00  0.00  0.00  1  119.9750000  -171544.000
    200.000  600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9641.000
-2.506864207D+05 3.294827830D+03-1.713873471D+01 8.733851000D-02-1.306227449D-04
  7.362001640D-08 0.000000000D+00          -3.800873290D+04 9.277002410D+01
    600.000  1400.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          9641.000
  9.114353860D+05-5.471736420D+03 2.097363178D+01-1.514620285D-02 1.275975810D-05
-4.881556790D-09 7.710203910D-13          7.794979850D+03-1.227198763D+02
Fe2O3(cr)          Hematite below Curie pt. Pankratz,1983 p158.
  2 g 1/01 FE  2.00O  3.00  0.00  0.00  0.00  1  159.6882000  -824248.000
    298.150  600.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
-2.713211885D+06 2.323047773D+04-6.765701770D+01 1.306052231D-01-6.970688120D-05
  0.000000000D+00 0.000000000D+00          -2.256089397D+05 4.228072580D+02
    600.000  960.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
  3.333492510D+08-1.859961832D+06 3.885138190D+03-3.562599480D+00 1.231055904D-03
  0.000000000D+00 0.000000000D+00          1.058058870D+07-2.555306055D+04
Fe2O3(cr)          Hematite above Curie pt. Pankratz,1983 p158.
  2 g 1/01 FE  2.00O  3.00  0.00  0.00  0.00  2  159.6882000  -824248.000
    960.000  1800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
-2.84409066D+07 1.253786450D+05-2.119080355D+02 2.221481558D-01-1.206765164D-04
  3.480738050D-08-4.165297860D-12          -8.483926520D+05 1.433002161D+03
    1800.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
  0.000000000D+00 0.000000000D+00 1.711439880D+01 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00          -1.041599645D+05-8.780613745D+01
Fe2(SO4)3(cr)      Chase,1998 p1249.
  2 j 6/66 FE  2.00S  3.00O  12.00  0.00  0.00  1  399.8778000  -2582992.400
    298.150  700.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
-3.987499800D+06 4.471584410D+04-1.871627045D+02 5.203843270D-01-5.255167310D-04
  2.053709591D-07 0.000000000D+00          -5.418976280D+05 1.097303717D+03
    700.000  2000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          0.000
-1.749475174D+07 7.308320780D+04-9.392951360D+01 1.468051405D-01-7.963099160D-05
  2.311696556D-08-2.739014918D-12          -7.607146510D+05 6.865330290D+02
Fe3O4(cr)          Magnetite. Pankratz,1983 p160. Westrum,1969.
  3 g 1/01 FE  3.00O  4.00  0.00  0.00  0.00  1  231.5326000  -1118383.200
    200.000  298.1507 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24762.073
-5.182671230D+07 1.293463453D+06-1.341121962D+04 7.401842440D+01-2.285725885D-01
  3.752884300D-04-2.559338368D-07          -5.570751240D+06 6.575689710D+04
    298.150  800.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24762.073
-4.407671380D+06 5.351760270D+04-2.613667759D+02 7.431931490D-01-9.767843990D-04
  5.858865440D-07-8.780843180D-11          -4.018075450D+05 1.478276107D+03
    800.000  850.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24762.073
  0.000000000D+00 0.000000000D+00-1.070116148D+02 1.738436706D-01 0.000000000D+00
  0.000000000D+00 0.000000000D+00          -9.231022600D+04 6.169265720D+02
Fe3O4(cr)          Magnetite above Curie Pt. Pankratz,1983 p160.
  1 g 1/01 FE  3.00O  4.00  0.00  0.00  0.00  2  231.5326000  -1118383.200
    850.000  1870.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24762.073
  5.731691980D+07-1.816105186D+05 2.777813396D+02-1.849830315D-01 6.145641150D-05
-3.660350860D-09-1.383713617D-12          9.906992850D+05-1.868855147D+03
Fe3O4(L)          Liquid. Chase,1998 p1250 6/65.
  1 g 1/01 FE  3.00O  4.00  0.00  0.00  0.00  3  231.5326000  -1118383.200
    1870.000  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          24762.073
  0.000000000D+00 0.000000000D+00 2.415439996D+01 0.000000000D+00 0.000000000D+00
  0.000000000D+00 0.000000000D+00          -1.242541349D+05-1.109781572D+02
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  69.7230000  0.000
    100.000  302.9207 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5640.000
  1.665524651D+03-1.667535996D+02 3.860876380D+00-1.325442179D-03 2.405494396D-06
  0.000000000D+00 0.000000000D+00          -1.577791876D+02-1.730178030D+01
Ga(L)            Liquid. Ref-Elm. Gurvich,1996a pt1 p209 pt2 p169.
  1 tpis96 GA  1.00  0.00  0.00  0.00  0.00  2  69.7230000  0.000
    302.920  6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          5640.000
  2.846830421D+04 0.000000000D+00 3.135362156D+00-3.620177256D-05 2.898547239D-08
  0.000000000D+00 0.000000000D+00          -1.716496723D+02-1.053717280D+01
GaBr3(cr)         Gurvich,1996a pt1 p242 pt2 p195.
  1 tpis96 GA  1.00BR  3.00  0.00  0.00  0.00  1  309.4350000  -387000.000
    298.150  397.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          25000.000
  0.000000000D+00 0.000000000D+00 3.563409028D+00 2.798433101D-02 0.000000000D+00
  0.000000000D+00 0.000000000D+00          -4.885137800D+04-6.997495329D+00

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## Appendix D (continued)

GaBr<sub>3</sub>(L) Liquid. Gurvich,1996a pt1 p242 pt2 p195.  
 1 tps96 GA 1.00BR 3.00 0.00 0.00 0.00 2 309.4350000 -387000.000  
 397.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 25000.000  
 0.000000000D+00 0.000000000D+00 1.544288238D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.990695050D+04-6.330801668D+01

GaCl<sub>3</sub>(cr) Triclinic. Gurvich,1996a pt1 p234 pt2 p188.  
 1 tps96 GA 1.00CL 3.00 0.00 0.00 0.00 1 176.0820000 -527000.000  
 298.150 351.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20000.000  
 0.000000000D+00 0.000000000D+00 2.725476306D+00 2.958442530D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.551070110D+04-8.232857519D+00

GaCl<sub>3</sub>(L) Liquid. Gurvich,1996a pt1 p234 pt2 p188.  
 1 tps96 GA 1.00CL 3.00 0.00 0.00 0.00 2 176.0820000 -527000.000  
 351.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20000.000  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.599449360D+04-5.489418092D+01

GaF<sub>3</sub>(cr) Hexagonal. Gurvich,1996a pt1 p226 pt2 p181.  
 1 tps96 GA 1.00F 3.00 0.00 0.00 0.00 1 126.7182096 -1175000.000  
 298.150 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16700.000  
 0.000000000D+00 0.000000000D+00 9.361585950D+00 4.503211855D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.443105216D+05-4.313509369D+01

GaI<sub>3</sub>(cr) Rhombic. Gurvich,1996a pt1 p249 pt2 p202.  
 1 tps96 GA 1.00I 3.00 0.00 0.00 0.00 1 450.4364100 -218000.000  
 298.150 485.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29000.000  
 0.000000000D+00 0.000000000D+00 6.461715723D+00 1.866676449D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.897546082D+04-1.772605384D+01

GaI<sub>3</sub>(L) Liquid. Gurvich,1996a pt1 p249 pt2 p202.  
 1 tps96 GA 1.00I 3.00 0.00 0.00 0.00 2 450.4364100 -218000.000  
 485.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29000.000  
 0.000000000D+00 0.000000000D+00 1.656140891D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.012686264D+04-6.793170105D+01

Ga<sub>2</sub>O<sub>3</sub>(cr) Monoclinic. Gurvich,1996a pt1 p219 pt2 p176.  
 2 tps96 GA 2.000 3.00 0.00 0.00 0.00 1 187.4442000 -1091000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14550.000  
 -1.515635939D+07 2.787922412D+05-2.090093764D+03 8.236854680D+00-1.771414598D-02  
 1.991804320D-05-9.167934200D-09 -1.391968792D+06 1.094221304D+04  
 500.000 2080.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14550.000  
 -2.857534599D+05 0.000000000D+00 1.375883846D+01 1.799504721D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.363570445D+05-7.032081677D+01

Ga<sub>2</sub>O<sub>3</sub>(L) Liquid. Gurvich,1996a pt1 p219 pt2 p176.  
 1 tps96 GA 2.000 3.00 0.00 0.00 0.00 3 187.4442000 -1091000.000  
 2080.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14550.000  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.317078351D+05-1.026657694D+02

Ge(cr) Cubic. Ref-Elm. Gurvich,1991 pt1 p308 pt2 p268.  
 2 tps91 GE 1.00 0.00 0.00 0.00 0.00 1 72.6400000 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 tps91 GE 1.00 0.00 0.00 0.00 0.00 2 72.6400000 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

GeO<sub>2</sub>(II) Tetragonal Rutile, Gurvich,1991 pt1 p319 pt2 p275.  
 2 tps91 GE 1.000 2.00 0.00 0.00 0.00 1 104.6388000 -580200.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7230.400  
 -1.362061010D+04 0.000000000D+00 1.390091028D+00 1.608814892D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.095682740D+04-8.017483700D+00  
 298.150 1308.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7230.400  
 -2.763121338D+05 0.000000000D+00 9.404643208D+00-1.212218158D-03 1.110107511D-06  
 0.000000000D+00 0.000000000D+00 -7.346830070D+04-5.004997052D+01

GeO<sub>2</sub>(I) Hexagonal alpha-quartz, Gurvich,1991 pt1 p319 pt2 p275.  
 1 tps91 GE 1.000 2.00 0.00 0.00 0.00 3 104.6388000 -580200.000  
 1308.000 1388.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7230.400  
 -1.535267863D+05 0.000000000D+00 7.481860025D+00 1.711465859D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.994652970D+04-3.711331960D+01

## Appendix D (continued)

GeO<sub>2</sub> (L) Tetragonal liquid, Gurvich, 1991 pt1 p319 pt2 p275.  
 1 tpis91 GE 1.000 2.00 0.00 0.00 0.00 4 104.6388000 -580200.000  
 1388.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7230.400  
 0.000000000D+00 0.000000000D+00 9.441326067D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.883837870D+04-4.738551165D+01

GeS (cr) Crystal (II). Gurvich, 1991 pt1 p342 pt2 p296.  
 2 tpis91 GE 1.00S 1.00 0.00 0.00 0.00 1 104.7050000 -75348.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9657.400  
 -1.753890915D+04 0.000000000D+00 4.967049230D+00 3.277123440D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.074763864D+04-2.138030847D+01  
 298.150 931.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9657.400  
 0.000000000D+00 0.000000000D+00 5.015328624D+00 2.453542061D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.066660187D+04-2.131118286D+01

GeS (L) Liquid. Gurvich, 1991 pt1 p342 pt2 p296.  
 1 tpis91 GE 1.00S 1.00 0.00 0.00 0.00 3 104.7050000 -75348.000  
 931.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9657.400  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.874413010D+03-3.707715519D+01

GeS<sub>2</sub> (II) Crystal II. Gurvich, 1991 pt1 p345 pt2 p298.  
 2 tpis91 GE 1.00S 2.00 0.00 0.00 0.00 1 136.7700000 -121500.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12750.300  
 -2.239538329D+04 0.000000000D+00 5.754200020D+00 8.048243800D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.676145505D+04-2.405323435D+01  
 298.150 1113.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12750.300  
 -3.367606750D+04 0.000000000D+00 7.889821529D+00 1.310961199D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.713657615D+04-3.427587425D+01

GeS<sub>2</sub> (L) Liquid. Gurvich, 1991 pt1 p345 pt2 p298.  
 1 tpis91 GE 1.00S 2.00 0.00 0.00 0.00 2 136.7700000 -121500.000  
 1113.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12750.300  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.893876733D+04-6.006450099D+01

HBO<sub>2</sub> (cr) Crystal, metaboric acid. Gurvich, 1996a pt1 p41 pt2 p25.  
 1 tpis96 H 1.00B 1.000 2.00 0.00 0.00 1 43.8177400 -804600.000  
 298.150 509.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8460.200  
 0.000000000D+00 0.000000000D+00 4.478916978D+00 7.045514408D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.841912440D+04-2.172637097D+01

HBO<sub>2</sub> (L) Liquid, metaboric acid. Gurvich, 1996a pt1 p41 pt2 p25.  
 1 tpis96 H 1.00B 1.000 2.00 0.00 0.00 2 43.8177400 -804600.000  
 509.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8460.200  
 0.000000000D+00 0.000000000D+00 1.262852531D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.993471070D+04-6.555326576D+01

H<sub>2</sub>O (cr) Ice. Gordon, 1982.  
 1 g11/99 H 2.000 1.00 0.00 0.00 0.00 1 18.0152800 -299108.000  
 200.000 273.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -4.026777480D+05 2.747887946D+03 5.738336630D+01-8.267915240D-01 4.413087980D-03  
 -1.054251164D-05 9.694495970D-09 -5.530314990D+04-1.902572063D+02

H<sub>2</sub>O (L) Liquid. Cox, 1989. Haar, 1984. Keenan, 1984. Stimson, 1969.  
 2 g 8/01 H 2.000 1.00 0.00 0.00 0.00 2 18.0152800 -285830.000  
 273.150 373.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13278.000  
 1.326371304D+09-2.448295388D+07 1.879428776D+05-7.678995050D+02 1.761556813D+00  
 -2.151167128D-03 1.092570813D-06 1.101760476D+08-9.779700970D+05  
 373.150 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13278.000  
 1.263631001D+09-1.680380249D+07 9.278234790D+04-2.722373950D+02 4.479243760D-01  
 -3.919397430D-04 1.425743266D-07 8.113176880D+07-5.134418080D+05

H<sub>2</sub>SO<sub>4</sub> (L) Chase, 1998 p1335.  
 1 j 9/77 H 2.00S 1.000 4.00 0.00 0.00 1 98.0784800 -813988.832  
 283.456 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28226.000  
 -7.749933850D+04 1.040538662D+03 4.433804910D+00 3.648845480D-02-1.743440132D-05  
 1.175631937D-08-3.170091690D-12 -1.068997367D+05-1.353966639D+01

H<sub>3</sub>BO<sub>3</sub> (cr) Triclinic, orthoboric acid. Gurvich, 1996a pt1 p48 pt2 p31.  
 1 tpis96 H 3.00B 1.000 3.00 0.00 0.00 1 61.8330200 -1094800.000  
 200.000 444.1007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13520.430  
 2.370260101D+06-3.116426553D+04 1.488140666D+02-2.710868145D-01 2.274904549D-04  
 0.000000000D+00 0.000000000D+00 1.950811769D+04-8.575441950D+02

H<sub>3</sub>BO<sub>3</sub> (L) Liquid, orthoboric acid. Gurvich, 1996a pt1 p48 pt2 p31.  
 1 tpis96 H 3.00B 1.000 3.00 0.00 0.00 2 61.8330200 -1094800.000  
 444.100 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13520.430  
 0.000000000D+00 0.000000000D+00 2.164890054D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.367426553D+05-1.100910256D+02



## Appendix D (continued)

H3PO4(cr) Crystal, Phosphoric acid. Chase, 1998 p1345-7.  
 1 j12/71 H 3.00P 1.000 4.00 0.00 0.00 1 97.9951810 -1284488.000  
 200.000 315.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16980.000  
 2.733365471D+03 0.000000000D+00 1.109347863D+00 4.129024570D-02 -7.810353320D-06  
 0.000000000D+00 0.000000000D+00 -1.565753156D+05 -4.973473130D+00

H3PO4(L) Liquid, Phosphoric acid. Chase, 1998 pp1345-7.  
 1 j12/71 H 3.00P 1.000 4.00 0.00 0.00 2 97.9951810 -1284488.000  
 315.500 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16980.000  
 4.109081110D+04 -4.410343500D+02 8.547791650D+00 3.198261330D-02 5.167529530D-06  
 -3.256216600D-09 8.323148740D-13 -1.543175380D+05 -4.155398650D+01

Hg(cr) Tetragonal. Ref-Elm. Chase, 1998 pp1373-4.  
 1 j12/61 HG 1.00 0.00 0.00 0.00 0.00 1 200.5900000 0.000  
 100.000 234.2907 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9343.000  
 -3.184586610D+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 pp1373-4.  
 2 j12/61 HG 1.00 0.00 0.00 0.00 0.00 2 200.5900000 0.000  
 234.290 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9343.000  
 1.058325418D+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

HgBr2(cr) Chase, 1998 p482 3/62. Pankratz, 1984 p302.  
 1 g12/00 HG 1.00BR 2.00 0.00 0.00 0.00 1 360.3980000 -175309.600  
 298.150 514.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -1.853158540D+06 2.003808568D+04 -7.235875200D+01 1.451267662D-01 -9.240269430D-05  
 0.000000000D+00 0.000000000D+00 -1.255295454D+05 4.503769710D+02

HgBr2(L) Chase, 1998 pp482-4 3/62.  
 1 g12/00 HG 1.00BR 2.00 0.00 0.00 0.00 2 360.3980000 -175309.600  
 514.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 1.227853475D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.320342036D+04 -4.684603799D+01

HgO(cr) Chase, 1998 p1382.  
 2 j 6/62 HG 1.000 1.00 0.00 0.00 0.00 1 216.5894000 -90789.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9104.000  
 -1.062935837D+04 0.000000000D+00 3.345782860D+00 8.775373380D-03 -6.110417750D-06  
 0.000000000D+00 0.000000000D+00 -1.228859467D+04 -1.301600791D+01  
 400.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9104.000  
 1.582008299D+06 -1.511620794D+04 6.157172990D+01 -1.075963114D-01 1.203602940D-04  
 -7.037671400D-08 1.672097585D-11 6.599870400D+04 -3.568628600D+02

I2(cr) Rhombic. Ref-Elm. Gurvich, 1989 pt1 p219 pt2 p315.  
 1 tpis89 I 2.00 0.00 0.00 0.00 0.00 1 253.8089400 0.000  
 200.000 386.7507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13196.000  
 -3.901269140D+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 2 253.8089400 0.000  
 386.750 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13196.000  
 0.000000000D+00 0.000000000D+00 9.568212679D+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, 1996a pt1 255 pt2 p207.  
 1 tpis96 IN 1.00 0.00 0.00 0.00 0.00 1 114.8180000 0.000  
 100.000 429.7847 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6610.080  
 8.511616870D+03 -3.450470040D+02 6.838785170D+00 -1.818530679D-02 4.122421420D-05  
 -2.960008730D-08 0.000000000D+00 4.580589980D+02 -2.928914154D+01

In(L) Liquid. Ref-Elm. Gurvich, 1996a pt1 255 pt2 p207.  
 1 tpis96 IN 1.00 0.00 0.00 0.00 0.00 2 114.8180000 0.000  
 429.784 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6610.080  
 5.092302493D+04 0.000000000D+00 3.302178962D+00 -1.313366633D-04 6.037637816D-08  
 0.000000000D+00 0.000000000D+00 -4.511517590D+02 -1.075015830D+01

InBr(cr) Rhombic Gurvich, 1996a pt1 p289 pt2 p232.  
 1 tpis96 IN 1.00BR 1.00 0.00 0.00 0.00 1 194.7220000 -175000.000  
 298.150 558.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12200.000  
 0.000000000D+00 0.000000000D+00 4.633586345D+00 4.628534935D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.263476911D+04 -1.455042037D+01

InBr(L) Liquid Gurvich, 1996a pt1 p289 pt2 p232  
 1 tpis96 IN 1.00BR 1.00 0.00 0.00 0.00 2 194.7220000 -175000.000  
 558.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12200.000  
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.222238473D+04 -3.267500998D+01

## Appendix D (continued)

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InBr3(cr)          Gurvich,1996a pt1 p292 pt2 p235.
  1 tps96 IN  1.00BR  3.00  0.00  0.00  0.00  1  354.5300000  -399000.000
    298.150    693.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      24500.000
    0.000000000D+00 0.000000000D+00 1.154114915D+01 2.436824299D-03 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -5.153769860D+04-4.543581045D+01
InBr3(L)          Liquid Gurvich,1996a pt1 p292 pt2 p235.
  1 tps96 IN  1.00BR  3.00  0.00  0.00  0.00  2  354.5300000  -399000.000
    693.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      24500.000
    0.000000000D+00 0.000000000D+00 1.623667540D+01 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -5.107949370D+04-6.994831229D+01
InCL(crII)        Cubic Gurvich,1996a pt1 p280 pt2 p224.
  1 tps96 IN  1.00CL  1.00  0.00  0.00  0.00  1  150.2710000  -186500.000
    298.150    387.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12400.000
    0.000000000D+00 0.000000000D+00 5.163984408D+00 3.438567035D-03 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -2.412314134D+04-1.842034240D+01
InCL(crI)         Rhombic Gurvich,1996a pt1 p280 pt2 p224.
  1 tps96 IN  1.00CL  1.00  0.00  0.00  0.00  2  150.2710000  -186500.000
    387.000    484.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12400.000
    0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -2.441117035D+04-2.629006183D+01
InCL(L)          Liquid Gurvich,1996a pt1 p280 pt2 p224
  1 tps96 IN  1.00CL  1.00  0.00  0.00  0.00  3  150.2710000  -186500.000
    484.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      12400.000
    0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -2.248971016D+04-2.917594080D+01
InCl3(cr)         Monoclinic Gurvich,1996a pt1 p284 pt2 p227.
  1 tps96 IN  1.00CL  3.00  0.00  0.00  0.00  1  221.1770000  -530000.000
    298.150    856.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      21000.000
    0.000000000D+00 0.000000000D+00 1.093437857D+01 3.665158861D-03 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -6.716697410D+04-4.631386948D+01
InCl3(L)          Liquid Gurvich,1996a pt1 p284 pt2 p227.
  1 tps96 IN  1.00CL  3.00  0.00  0.00  0.00  2  221.1770000  -530000.000
    856.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      21000.000
    0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -6.526246230D+04-6.056749656D+01
InF3(cr)          Hexagonal Gurvich,1996a pt1 p274 pt2 p219.
  1 tps96 IN  1.00F   3.00  0.00  0.00  0.00  1  171.8132096  -1190000.000
    298.150    1445.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19400.000
    0.000000000D+00 0.000000000D+00 9.751747247D+00 4.404348542D-03 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -1.462265291D+05-4.364479594D+01
InF3(L)          Liquid Gurvich,1996a pt1 p274 pt2 p219.
  1 tps96 IN  1.00F   3.00  0.00  0.00  0.00  2  171.8132096  -1190000.000
    1445.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19400.000
    0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -1.431278760D+05-7.826197980D+01
InI(cr)           Rhombic Gurvich,1996a pt1 p296 pt2 p240
  1 tps96 IN  1.00I   1.00  0.00  0.00  0.00  1  241.7224700  -102500.000
    200.000    637.5007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      13354.000
-9.253976720D+04 1.215133840D+03-1.038882859D-02 1.368794477D-02-9.117964390D-06
  1.596277777D-09 1.519819589D-12      -2.009017203D+04 1.436598613D+01
InI(L)           Liquid Gurvich,1996a pt1 p296 pt2 p240
  1 tps96 IN  1.00I   1.00  0.00  0.00  0.00  2  241.7224700  -102500.000
    637.500    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      13354.000
    0.000000000D+00 0.000000000D+00 8.443071209D+00 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -1.331949891D+04-3.168475714D+01
InI2(crII)        Gurvich,1996a pt1 p299 pt2 p242.
  1 tps96 IN  1.00I   2.00  0.00  0.00  0.00  1  368.6269400  -176000.000
    200.000    428.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19197.000
  2.657410907D+04 0.000000000D+00 6.946210170D+00 6.889884760D-03 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -2.345592914D+04-2.056620828D+01
InI2(crI)         Gurvich,1996a pt1 p299 pt2 p242.
  1 tps96 IN  1.00I   2.00  0.00  0.00  0.00  2  368.6269400  -176000.000
    428.000    497.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19197.000
    0.000000000D+00 0.000000000D+00 1.080520680D+01 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -2.438345996D+04-4.070950647D+01
InI2(L)           Liquid Gurvich,1996a pt1 p299 pt2 p242.
  1 tps96 IN  1.00I   2.00  0.00  0.00  0.00  3  368.6269400  -176000.000
    497.000    6000.0007 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0      19197.000
    0.000000000D+00 0.000000000D+00 1.379516051D+01 0.000000000D+00 0.000000000D+00
    0.000000000D+00 0.000000000D+00      -2.444424767D+04-5.640525880D+01

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## Appendix D (continued)

InI3(cr) Monoclinic Gurvich,1996a pt1 p301 pt2 p244.  
 1 tps96 IN 1.00I 3.00 0.00 0.00 0.00 1 495.5314100 -224000.000  
 296.000 480.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29888.000  
 -1.888265213D+03 0.000000000D+00 1.096468704D+01 4.804492387D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.042985260D+04-3.708283570D+01

InI3(L) Liquid Gurvich,1996a pt1 p301 pt2 p244.  
 1 tps96 IN 1.00I 3.00 0.00 0.00 0.00 2 495.5314100 -224000.000  
 480.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29888.000  
 0.000000000D+00 0.000000000D+00 1.652532741D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.031892811D+04-6.447232654D+01

In2O3(cr) Cubic. Gurvich,1996a pt1 p267 pt2 p214.  
 2 tps96 IN 2.00O 3.00 0.00 0.00 0.00 1 277.6342000 -923000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16600.000  
 -9.503707350D+06 1.770907496D+05-1.344503703D+03 5.391303710D+00-1.171772659D-02  
 1.329195789D-05-6.163943540D-09 -9.104733670D+05 7.021339210D+03  
 500.000 2186.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16600.000  
 -2.719943809D+05 0.000000000D+00 1.461433085D+01 1.210173540D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.163340719D+05-7.291389772D+01

In2O3(L) Liquid. Gurvich,1996a pt1 p267 pt2 p214.  
 1 tps96 IN 2.00O 3.00 0.00 0.00 0.00 2 277.6342000 -923000.000  
 2186.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16600.000  
 0.000000000D+00 0.000000000D+00 1.924346714D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.108089477D+05-1.000602622D+02

K(cr) Cubic. Ref-Elm. Cox,1989 p257.  
 1 coda89 K 1.00 0.00 0.00 0.00 0.00 1 39.0983000 0.000  
 200.000 336.8607 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7088.000  
 -1.022031747D+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 p257.  
 1 coda89 K 1.00 0.00 0.00 0.00 0.00 2 39.0983000 0.000  
 336.860 2200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7088.000  
 -3.935722030D+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

KAlO2(II) Cubic Gurvich,1982 pt1 p416 pt2 p440.  
 2 tps82 K 1.00AL 1.00O 2.00 0.00 0.00 1 98.0786380 -1130600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13355.000  
 -4.112581400D+06 7.776836810D+04-5.971614160D+02 2.439288137D+00-5.340052400D-03  
 6.098541950D-06-2.843205389D-09 -4.867714660D+05 3.112191530D+03  
 500.000 810.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13355.000  
 -1.565945988D+05 0.000000000D+00 9.609859180D+00 4.379778490D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.395641536D+05-4.665045360D+01

KAlO2(I) Cubic Gurvich,1982 pt1 p416 pt2 p440.  
 1 tps82 K 1.00AL 1.00O 2.00 0.00 0.00 2 98.0786380 -1130600.000  
 810.000 1986.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13355.000  
 8.202527870D+05 0.000000000D+00 7.962706161D+00 3.725414967D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.366535595D+05-3.415265795D+01

KAlO2(L) Liquid. Gurvich,1982 pt1 p416 pt2 p440.  
 1 tps82 K 1.00AL 1.00O 2.00 0.00 0.00 3 98.0786380 -1130600.000  
 1986.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13355.000  
 0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.350952219D+05-8.015693620D+01

KBO2(cr) Hexagonal. Gurvich,1982 pt1 p414 pt2 p438.  
 2 tps82 K 1.00B 1.00O 2.00 0.00 0.00 1 81.9081000 -983000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12114.000  
 -1.601790683D+07 2.997219831D+05-2.274223151D+03 9.014942220D+00-1.951702277D-02  
 2.207384968D-05-1.021270864D-08 -1.468642542D+06 1.188723021D+04  
 500.000 1220.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12114.000  
 -2.328709444D+05 0.000000000D+00 9.862977090D+00 2.740064145D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.220704116D+05-4.870043770D+01

KBO2(L) Liquid. Gurvich,1982 pt1 p414 pt2 p438.  
 1 tps82 K 1.00B 1.00O 2.00 0.00 0.00 2 81.9081000 -983000.000  
 1220.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12114.000  
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.250545034D+05-9.581938648D+01

## Appendix D (continued)

KBr(cr) Cubic. Gurvich,1982 pt1 p394 pt2 p422.  
 2 tps82 K 1.00BR 1.00 0.00 0.00 0.00 1 119.0023000 -393450.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12210.000  
 5.931068110D+06-1.101548735D+05 8.346526100D+02-3.241060370D+00 6.976184850D-03  
 -7.847251340D-06 3.614707700D-09 4.475606580D+05-4.361638690D+03  
 500.000 1007.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12210.000  
 3.145485337D+04 0.000000000D+00 5.199966220D+00 2.540382104D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.887872000D+04-1.867132005D+01

KBr(L) Liquid. Gurvich,1982 pt1 p394 pt2 p422.  
 1 tps82 K 1.00BR 1.00 0.00 0.00 0.00 2 119.0023000 -393450.000  
 1007.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12210.000  
 0.000000000D+00 0.000000000D+00 8.358881040D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.773361440D+04-3.492371367D+01

KCN(II) Chase,1998 pp617-9.  
 2 j 3/66 K 1.00C 1.00N 1.00 0.00 0.00 1 65.1157000 -113470.000  
 168.300 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17343.000  
 4.789226660D+04-6.869399420D+02 1.189656301D+01-9.957932230D-03 9.253758250D-06  
 0.000000000D+00 0.000000000D+00 -1.275880363D+04-5.189047360D+01  
 400.000 895.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17343.000  
 -8.550726080D+04 7.115109180D+02 5.642442360D+00 3.733592200D-03-2.880609857D-06  
 8.848387980D-10 0.000000000D+00 -1.981154134D+04-1.586461470D+01

KCN(L) Chase,1998 pp617-9.  
 1 j 3/66 K 1.00C 1.00N 1.00 0.00 0.00 2 65.1157000 -113470.000  
 895.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17343.000  
 0.000000000D+00 0.000000000D+00 9.057899984D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.522666331D+04-3.545330543D+01

KCL(cr) Cubic. Gurvich,1982 pt1 p390 pt2 p419.  
 2 tps82 K 1.00CL 1.00 0.00 0.00 0.00 1 74.5513000 -436490.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11370.000  
 1.179895024D+06-2.217824961D+04 1.730930630D+02-6.545434150D-01 1.415897824D-03  
 -1.598259237D-06 7.387534150D-10 4.560782730D+04-8.991527150D+02  
 500.000 1044.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11370.000  
 2.888789664D+02 0.000000000D+00 5.287088550D+00 4.004092160D-03-4.343449010D-06  
 2.753186288D-09 0.000000000D+00 -5.421785640D+04-2.121648362D+01

KCL(L) Liquid. Gurvich,1982 pt1 p390 pt2 p419.  
 1 tps82 K 1.00CL 1.00 0.00 0.00 0.00 2 74.5513000 -436490.000  
 1044.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11370.000  
 0.000000000D+00 0.000000000D+00 8.659560215D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.322113230D+04-3.876839685D+01

KF(cr) Cubic. Gurvich,1982 pt1 p387 pt2 p416.  
 2 tps82 K 1.00F 1.00 0.00 0.00 0.00 1 58.0967032 -569900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10000.000  
 -2.920039956D+06 5.319604560D+04-3.910182930D+02 1.542524798D+00-3.296460120D-03  
 3.692487030D-06-1.695192481D-09 -3.107774664D+05 2.055199175D+03  
 500.000 1131.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10000.000  
 -3.379466710D+04 0.000000000D+00 5.806099490D+00 1.562870483D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.045670350D+04-2.573881635D+01

KF(L) Liquid. Gurvich,1982 pt1 p387 pt2 p416.  
 1 tps82 K 1.00F 1.00 0.00 0.00 0.00 2 58.0967032 -569900.000  
 1131.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10000.000  
 0.000000000D+00 0.000000000D+00 8.455098376D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.905565270D+04-3.960518579D+01

KH(cr) Cubic. Gurvich,1982 pt1 p381 pt2 p411.  
 1 tps82 K 1.00H 1.00 0.00 0.00 0.00 1 40.1062400 -57820.000  
 298.150 892.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7800.000  
 -6.457385920D+04 0.000000000D+00 4.092965190D+00 3.996988400D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.568660280D+03-1.870503989D+01

KH(L) Liquid. Gurvich,1982 pt1 p381 pt2 p411.  
 1 tps82 K 1.00H 1.00 0.00 0.00 0.00 2 40.1062400 -57820.000  
 892.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7800.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.737318610D+03-3.021766413D+01

K(HF2)(a) Alpha. Chase,1998 pp1104-6.  
 1 j 6/71 K 1.00H 1.00F 2.00 0.00 0.00 1 78.1030464 -931232.880  
 200.000 469.8507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15294.000  
 2.015718998D+03-3.533789190D+02 8.928247670D+00 2.814397451D-03 7.299809050D-06  
 0.000000000D+00 0.000000000D+00 -1.128323001D+05-4.066701520D+01

## Appendix D (continued)

K(HF2) (b)                      Beta.      Chase,1998 pp1104-6.  
 1 j 6/71 K    1.00H    1.00F    2.00    0.00    0.00 2    78.1030464    -931232.880  
               469.850    511.9507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    15294.000  
 0.000000000D+00 0.000000000D+00 1.205711461D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -1.145682138D+05-5.416912090D+01

K(HF2) (L)                      Liquid. Chase,1998 pp1104-6.  
 1 j 6/71 K    1.00H    1.00F    2.00    0.00    0.00 3    78.1030464    -931232.880  
               511.950    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    15294.000  
 0.000000000D+00 0.000000000D+00 1.258041665D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -1.140400401D+05-5.587860571D+01

KI(cr)                              Cubic. Gurvich,1982 pt1 p398 pt2 p425.  
 2 tps82 K    1.00I    1.00    0.00    0.00    0.00 1    166.0027700    -329300.000  
               200.000    500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12700.000  
 3.849118670D+06-7.198411950D+04 5.507582640D+02-2.141022674D+00 4.628312070D-03  
 -5.222322770D-06 2.411694600D-09                      2.826852967D+05-2.871024327D+03  
               500.000    954.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12700.000  
 2.770577458D+04 0.000000000D+00 5.235901210D+00 2.694044229D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -4.119339520D+04-1.772462446D+01

KI(L)                              Liquid. Gurvich,1982 pt1 p398 pt2 p425.  
 1 tps82 K    1.00I    1.00    0.00    0.00    0.00 2    166.0027700    -329300.000  
               954.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12700.000  
 0.000000000D+00 0.000000000D+00 8.455098376D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -4.017867910D+04-3.422733253D+01

KNO2(II)                           Hexagonal. Gurvich,1982 pt1 p404 pt2 p430.  
 1 tps82 K    1.00N    1.000    2.00    0.00    0.00 1    85.1038000    -365900.000  
               200.000    314.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22940.000  
 -1.228297484D+07 0.000000000D+00 1.182559906D+03-6.076842320D+00 8.778424840D-03  
 0.000000000D+00 0.000000000D+00                      -2.452424942D+05-5.366905900D+03

KNO2(I)                              Cubic. Gurvich,1982 pt1 p404 pt2 p430.  
 1 tps82 K    1.00N    1.000    2.00    0.00    0.00 2    85.1038000    -365900.000  
               314.700    711.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22940.000  
 0.000000000D+00 0.000000000D+00 9.827879214D+00 2.012866663D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -4.687774970D+04-3.782318671D+01

KNO2(L)                              Liquid. Gurvich,1982 pt1 p404 pt2 p430.  
 1 tps82 K    1.00N    1.000    2.00    0.00    0.00 3    85.1038000    -365900.000  
               711.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22940.000  
 0.000000000D+00 0.000000000D+00 1.226771030D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -4.609515960D+04-4.958866367D+01

KNO3(a)                              Rhombic. Gurvich,1982 pt1 p407 pt2 p432.  
 1 tps82 K    1.00N    1.000    3.00    0.00    0.00 1    101.1032000    -494000.000  
               200.000    402.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18750.000  
 3.565624070D+06-6.291319380D+04 4.392599940D+02-1.436497824D+00 2.380417773D-03  
 -1.518208824D-06 0.000000000D+00                      2.258505778D+05-2.341795728D+03

KNO3(b)                              Hexagonal. Gurvich,1982 pt1 p407 pt2 p432.  
 1 tps82 K    1.00N    1.000    3.00    0.00    0.00 2    101.1032000    -494000.000  
               402.000    607.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18750.000  
 3.211975210D+06 0.000000000D+00-5.032659772D+01 1.462070525D-01-8.159374395D-05  
 0.000000000D+00 0.000000000D+00                      -3.934846620D+04 2.807123740D+02

KNO3(L)                              Liquid. Gurvich,1982 pt1 p407 pt2 p432.  
 1 tps82 K    1.00N    1.000    3.00    0.00    0.00 3    101.1032000    -494000.000  
               607.700    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18750.000  
 0.000000000D+00 0.000000000D+00 1.695830542D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -6.345106350D+04-7.918784042D+01

KOH(a)                              Alpha,beta. Gurvich,1997 p1031.  
 1 g 8/97 K    1.00O    1.00H    1.00    0.00    0.00 1    56.1056400    -423400.000  
               100.000    298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12600.000  
 -4.380064620D+05 1.125472885D+04-1.023623342D+02 4.375630440D-01-5.920346390D-04  
 0.000000000D+00 0.000000000D+00                      -1.002155756D+05 5.241308280D+02

KOH(b)                              Beta.      Gurvich,1997 p1031.  
 1 g 8/97 K    1.00O    1.00H    1.00    0.00    0.00 2    56.1056400    -423400.000  
               298.150    517.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12600.000  
 -2.814357070D+03 0.000000000D+00 6.478313214D+00 6.183767895D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -5.313882160D+04-2.899826328D+01

KOH(c)                              Gamma.      Gurvich,1997 p1031.  
 1 g 8/97 K    1.00O    1.00H    1.00    0.00    0.00 3    56.1056400    -423400.000  
               517.000    679.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    12600.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00                      -5.325857830D+04-4.413346659D+01

## Appendix D (continued)

KOH(L) Liquid. Gurvich,1997 p1031.  
 1 g 8/97 K 1.000 1.00H 1.00 0.00 0.00 4 56.1056400 -423400.000  
 679.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12600.000  
 0.000000000D+00 0.000000000D+00 1.046363526D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.288008340D+04-4.822385687D+01

KO2(b) Tetragonal. Gurvich,1982 pt1 p375 pt2 p405.  
 1 tpis82 K 1.000 2.00 0.00 0.00 0.00 1 71.0971000 -283600.000  
 200.000 422.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16820.000  
 5.149174260D+06-7.614604350D+04 4.537181540D+02-1.295601160D+00 1.892822220D-03  
 -1.090404806D-06 0.000000000D+00 3.247518810D+05-2.484666478D+03

KO2(a) Cubic. Gurvich,1982 pt1 p375 pt2 p405.  
 1 tpis82 K 1.000 2.00 0.00 0.00 0.00 2 71.0971000 -283600.000  
 422.000 808.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16820.000  
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.734259730D+04-4.545206851D+01

KO2(L) Liquid. Gurvich,1982 pt1 p375 pt2 p405.  
 1 tpis82 K 1.000 2.00 0.00 0.00 0.00 3 71.0971000 -283600.000  
 808.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16820.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.603115500D+04-5.204773022D+01

K2CO3(a) Monoclinic. Gurvich,1982 pt1 p410 pt2 p434.  
 1 tpis82 K 2.00C 1.000 3.00 0.00 0.00 1 138.2055000 -1151500.000  
 200.000 693.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22665.000  
 -3.632826430D+05 5.957567840D+03-3.080710797D+01 1.494558714D-01-2.377158989D-04  
 2.231711601D-07-8.466662880D-11 -1.694136603D+05 1.763682121D+02

K2CO3(b) Hexagonal. Gurvich,1982 pt1 p410 pt2 p434.  
 1 tpis82 K 2.00C 1.000 3.00 0.00 0.00 2 138.2055000 -1151500.000  
 693.000 1173.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22665.000  
 0.000000000D+00 0.000000000D+00 1.310023080D+01 8.280944999D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.424065852D+05-5.805609552D+01

K2CO3(L) Liquid. Gurvich,1982 pt1 p410 pt2 p434.  
 1 tpis82 K 2.00C 1.000 3.00 0.00 0.00 3 138.2055000 -1151500.000  
 1173.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22665.000  
 0.000000000D+00 0.000000000D+00 2.471582811D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.466663988D+05-1.273064200D+02

K2O(c) III Cubic. Gurvich,1982 pt1 p377 pt2 p406.  
 1 tpis82 K 2.000 1.00 0.00 0.00 0.00 1 94.1960000 -361700.000  
 298.150 590.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13700.000  
 0.000000000D+00 0.000000000D+00 6.140710637D+00 8.448122619D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.570860710D+04-2.596002023D+01

K2O(b) II Cubic. Gurvich,1982 pt1 p377 pt2 p406.  
 1 tpis82 K 2.000 1.00 0.00 0.00 0.00 2 94.1960000 -361700.000  
 590.000 645.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13700.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.762703040D+04-5.838924536D+01

K2O(a) I Tetragonal. Gurvich,1982 pt1 p377 pt2 p406.  
 1 tpis82 K 2.000 1.00 0.00 0.00 0.00 3 94.1960000 -361700.000  
 645.000 1013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13700.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.714594370D+04-5.764337454D+01

K2O(L) Liquid. Gurvich,1982 pt1 p377 pt2 p406.  
 1 tpis82 K 2.000 1.00 0.00 0.00 0.00 4 94.1960000 -361700.000  
 1013.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13700.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.389860860D+04-5.443771306D+01

K2O2(cr) Rhombic. Gurvich,1982 pt1 p379 pt2 p409.  
 1 tpis82 K 2.000 2.00 0.00 0.00 0.00 1 110.1954000 -443000.000  
 298.150 818.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17000.000  
 0.000000000D+00 0.000000000D+00 9.151230800D+00 6.015267286D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.627614800D+04-3.986168914D+01

K2O2(L) Liquid. Gurvich,1982 pt1 p379 pt2 p409.  
 1 tpis82 K 2.000 2.00 0.00 0.00 0.00 2 110.1954000 -443000.000  
 818.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17000.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.749561030D+04-7.864151320D+01

## Appendix D (continued)

K2S(cr) Below lambda. Chase,1998 pp1486-8.

2 j 3/78 K	2.00S	1.00	0.00	0.00	0.00	1	110.2616000	-376560.000
298.150	600.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.724669150D+04	-4.465995260D+02	9.600035840D+00	7.836273870D-04	1.295338974D-06	0.000000000D+00	0.000000000D+00	-4.549501380D+04	-4.238203950D+01
600.000	1050.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.237549376D+09	-7.863379810D+06	1.968151557D+04	-2.415909047D+01	1.451020806D-02	-3.388041040D-06	0.000000000D+00	4.392639800D+07	-1.251401185D+05

K2S(cr) Above lambda. Chase,1998 pp1486-8.

2 j 3/78 K	2.00S	1.00	0.00	0.00	0.00	2	110.2616000	-376560.000
1050.000	1100.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.564212060D+02	-1.266383838D-01	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.311392922D+05	-9.279088390D+02
1100.000	1221.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.711898382D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-5.452307000D+04	-9.166848070D+01

K2S(L) Chase,1998 pp1486-8.

1 j 3/78 K	2.00S	1.00	0.00	0.00	0.00	3	110.2616000	-376560.000
1221.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.214261815D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-4.650451120D+04	-5.470849197D+01

K2SO4(II) Rhombic. Gurvich,1982 pt1 p402 pt2 p428.

2 tpis82 K	2.00S	1.000	4.00	0.00	0.00	1	174.2592000	-1437700.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
7.718871240D+06	-1.416712413D+05	1.060181562D+03	-4.031007910D+00	8.614683760D-03	-9.611228510D-06	4.397898620D-09	4.640403120D+05	-5.555950140D+03
500.000	857.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.858415070D+04	0.000000000D+00	1.165680854D+01	1.576835485D-02	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.772539211D+05	-5.027549500D+01

K2SO4(I) Hexagonal. Gurvich,1982 pt1 p402 pt2 p428.

1 tpis82 K	2.00S	1.000	4.00	0.00	0.00	2	174.2592000	-1437700.000
857.000	1342.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.683008379D+07	0.000000000D+00	-3.453625048D+01	4.086410384D-02	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.262250083D+05	2.527928284D+02

K2SO4(L) Liquid. Gurvich,1982 pt1 p402 pt2 p428.

1 tpis82 K	2.00S	1.000	4.00	0.00	0.00	3	174.2592000	-1437700.000
1342.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.405433393D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.762313671D+05	-1.157513010D+02

K2SiO3(cr) Rhombic. Gurvich,1982 pt1 p412 pt2 p436.

2 tpis82 K	2.00SI	1.000	3.00	0.00	0.00	1	154.2803000	-1543000.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.855673428D+06	-5.059971270D+04	3.647712840D+02	-1.277216470D+00	2.614874944D-03	-2.812883261D-06	1.248415754D-09	4.217450990D+04	-1.927446205D+03
500.000	1249.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.541934726D+05	0.000000000D+00	1.400996506D+01	6.254878280D-03	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.905514472D+05	-6.499565930D+01

K2SiO3(L) Liquid. Gurvich,1982 pt1 p412 pt2 p436.

1 tpis82 K	2.00SI	1.000	3.00	0.00	0.00	2	154.2803000	-1543000.000
1249.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.285161723D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	-1.941869756D+05	-1.182498589D+02

K2Si2O5(a) III. Gurvich,1982 pt1 p413 pt2 p437.

1 tpis82 K	2.00SI	2.000	5.00	0.00	0.00	1	214.3646000	-2505000.000
200.000	510.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.332332468D+07	2.509615155D+05	-1.911732601D+03	7.658564980D+00	-1.652056677D-02	1.854450564D-05	-8.489711240D-09	-1.432942804D+06	9.985815260D+03

K2Si2O5(b) II. Gurvich,1982 pt1 p413 pt2 p437.

1 tpis82 K	2.00SI	2.000	5.00	0.00	0.00	2	214.3646000	-2505000.000
510.000	867.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.201153165D+05	0.000000000D+00	1.900352516D+01	1.092379467D-02	0.000000000D+00	0.000000000D+00	0.000000000D+00	-3.078422822D+05	-8.941094441D+01

K2Si2O5(c) I. Gurvich,1982 pt1 p413 pt2 p437.

1 tpis82 K	2.00SI	2.000	5.00	0.00	0.00	3	214.3646000	-2505000.000
867.000	1318.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.696791513D+01	5.313602365D-04	0.000000000D+00	0.000000000D+00	0.000000000D+00	-3.105104930D+05	-1.339782607D+02

## Appendix D (continued)

K2Si2O5(L) Gurvich,1982 pt1 p413 pt2 p437.  
 1 tps82 K 2.00SI 2.000 5.00 0.00 0.00 4 214.3646000 -2505000.000  
 1318.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 28820.000  
 0.000000000D+00 0.000000000D+00 3.307470915D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.138641654D+05-1.739362353D+02

K3AlF6(II) Tetragonal. Gurvich,1982 pt1 p418 pt2 p442.  
 1 tps82 K 3.00AL 1.00F 6.00 0.00 0.00 1 258.2668572 -3347000.000  
 298.150 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 42600.000  
 0.000000000D+00 0.000000000D+00 1.838593014D+01 2.828982105D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.092884330D+05-7.891279947D+01

K3AlF6(I) Cubic. Gurvich,1982 pt1 p418 pt2 p442.  
 1 tps82 K 3.00AL 1.00F 6.00 0.00 0.00 2 258.2668572 -3347000.000  
 600.000 1273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 42600.000  
 0.000000000D+00 0.000000000D+00 2.893014742D+01 6.707551016D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.109483890D+05-1.321111106D+02

K3AlF6(L) Liquid. Gurvich,1982 pt1 p418 pt2 p442.  
 1 tps82 K 3.00AL 1.00F 6.00 0.00 0.00 3 258.2668572 -3347000.000  
 1273.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 42600.000  
 0.000000000D+00 0.000000000D+00 4.726676617D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.141107070D+05-2.430801826D+02

Li(cr) Crystal. Ref-Elm. Gurvich,1982 pt1 p245 pt2 p286.  
 2 tps82 LI 1.00 0.00 0.00 0.00 0.00 1 6.9410000 0.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4632.000  
 -9.860652350D+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 tps82 LI 1.00 0.00 0.00 0.00 0.00 2 6.9410000 0.000  
 453.690 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4632.000  
 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

LiAlO2(cr) Chase,1998 pp126-8.  
 2 j12/79 LI 1.00AL 1.000 2.00 0.00 0.00 1 65.9213380 -1188674.400  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9694.328  
 -2.403553110D+06 4.191135380D+04-2.947543676D+02 1.096024513D+00-2.070932308D-03  
 1.989368601D-06-7.643124070D-10 -3.359272460D+05 1.562056779D+03  
 700.000 1973.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9694.328  
 -1.440922218D+06 5.833386140D+03-1.030268470D+00 1.461691077D-02-7.831786240D-06  
 2.428705700D-09-3.067767899D-13 -1.811607791D+05 2.012864902D+01

LiAlO2(L) Chase,1998 pp126-8.  
 1 j12/79 LI 1.00AL 1.000 2.00 0.00 0.00 2 65.9213380 -1188674.400  
 1973.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9694.328  
 0.000000000D+00 0.000000000D+00 1.509649997D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.416553963D+05-8.099434263D+01

LiBO2(cr) Monoclinic. Gurvich,1982 pt1 p298 pt2 p331.  
 2 tps82 LI 1.00B 1.000 2.00 0.00 0.00 1 49.7508000 -1022900.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8880.000  
 -1.298972763D+02 2.476112547D+03-4.025475640D+01 2.755313951D-01-7.202835830D-04  
 9.355885600D-07-4.776147920D-10 -1.326385762D+05 1.863684915D+02  
 500.000 1122.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8880.000  
 -1.501059611D+05 0.000000000D+00 7.094387770D+00 5.990864950D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.259108022D+05-3.688511780D+01

LiBO2(L) Liquid. Gurvich,1982 pt1 p298 pt2 p331.  
 1 tps82 LI 1.00B 1.000 2.00 0.00 0.00 2 49.7508000 -1022900.000  
 1122.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8880.000  
 0.000000000D+00 0.000000000D+00 1.736722910D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.294550343D+05-9.861468152D+01

LiBr(cr) Cubic. Gurvich,1982 pt1 p284 pt2 p317.  
 2 tps82 LI 1.00BR 1.00 0.00 0.00 0.00 1 86.8450000 -351160.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10476.000  
 3.743262690D+06-7.020131930D+04 5.366833500D+02-2.085864954D+00 4.508762520D-03  
 -5.086004120D-06 2.348146084D-09 2.721051038D+05-2.801510974D+03  
 500.000 823.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10476.000  
 1.459008908D+04 0.000000000D+00 4.895008630D+00 3.134322823D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.378446420D+04-1.984092688D+01



## Appendix D (continued)

LiBr(L) Liquid. Gurvich,1982 pt1 p284 pt2 p317.  
 1 tps82 LI 1.00BR 1.00 0.00 0.00 0.00 2 86.8450000 -351160.000  
 823.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10476.000  
 0.000000000D+00 0.000000000D+00 7.853740028D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.305174650D+04 -3.455318466D+01

LiCl(cr) Cubic. Gurvich,1982 pt1 p279 pt2 p313.  
 2 tps82 LI 1.00CL 1.00 0.00 0.00 0.00 1 42.3940000 -408540.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9300.000  
 -2.180497685D+06 3.971320780D+04 -2.918258028D+02 1.160079971D+00 -2.482284097D-03  
 2.785692272D-06 -1.280897066D-09 -2.302427379D+05 1.533139994D+03  
 500.000 883.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9300.000  
 -3.595609330D+04 0.000000000D+00 5.480770500D+00 2.332209108D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.099411730D+04 -2.499631307D+01

LiCl(L) Liquid. Gurvich,1982 pt1 p279 pt2 p313.  
 1 tps82 LI 1.00CL 1.00 0.00 0.00 0.00 2 42.3940000 -408540.000  
 883.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9300.000  
 0.000000000D+00 0.000000000D+00 7.601169522D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.954114490D+04 -3.460716245D+01

LiF(cr) Cubic. Gurvich,1982 pt1 p273 pt2 p309.  
 2 tps82 LI 1.00F 1.00 0.00 0.00 0.00 1 25.9394032 -618300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6473.000  
 9.636751230D+05 -1.777983613D+04 1.305502564D+02 -4.624287950D-01 9.558363610D-04  
 -1.037162482D-06 4.637142460D-10 5.186488570D+03 -6.901111630D+02  
 500.000 1122.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6473.000  
 -7.420484740D+04 0.000000000D+00 5.359396170D+00 1.623955670D-03 2.090115068D-07  
 0.000000000D+00 0.000000000D+00 -7.628479220D+04 -2.715764184D+01

LiF(L) Liquid. Gurvich,1982 pt1 p273 pt2 p309.  
 1 tps82 LI 1.00F 1.00 0.00 0.00 0.00 2 25.9394032 -618300.000  
 1122.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6473.000  
 0.000000000D+00 0.000000000D+00 7.673332524D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.443734250D+04 -3.852218670D+01

LiH(cr) Cubic. Gurvich,1982 pt1 p263 pt2 p300.  
 1 tps82 LI 1.00H 1.00 0.00 0.00 0.00 1 7.9489400 -90650.000  
 200.000 965.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 3883.000  
 -7.983399540D+03 -4.135167420D+02 3.842672410D+00 3.568427660D-03 3.560726720D-07  
 9.299007330D-10 -5.466520940D-13 -9.882374510D+03 -2.193513588D+01

LiH(L) Liquid. Gurvich,1982 pt1 p263 pt2 p300.  
 1 tps82 LI 1.00H 1.00 0.00 0.00 0.00 2 7.9489400 -90650.000  
 965.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 3883.000  
 0.000000000D+00 0.000000000D+00 6.614941831D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.089088820D+04 -3.406734782D+01

LiI(cr) Cubic. Gurvich,1982 pt1 p287 pt2 p321.  
 2 tps82 LI 1.00I 1.00 0.00 0.00 0.00 1 133.8454700 -273200.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11360.000  
 -6.958662980D+04 4.035715450D+02 7.056546540D+00 -1.824255625D-02 6.907245220D-05  
 -9.841303530D-08 5.297565590D-11 -3.712485890D+04 -2.568066591D+01  
 500.000 742.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11360.000  
 0.000000000D+00 0.000000000D+00 5.248298340D+00 2.986457552D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.455573620D+04 -2.036433073D+01

LiI(L) Liquid. Gurvich,1982 pt1 p287 pt2 p321.  
 1 tps82 LI 1.00I 1.00 0.00 0.00 0.00 2 133.8454700 -273200.000  
 742.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11360.000  
 0.000000000D+00 0.000000000D+00 7.601169522D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.371867140D+04 -3.132631144D+01

LiNO2(II) Crystal. Gurvich,1982 pt1 p292 pt2 p326.  
 1 tps82 LI 1.00N 1.000 2.00 0.00 0.00 1 52.9465000 -368300.000  
 298.150 369.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12100.000  
 0.000000000D+00 0.000000000D+00 -1.026999787D+00 2.885846550D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.527251980D+04 7.831186054D+00

LiNO2(I) Hexagonal. Gurvich,1982 pt1 p292 pt2 p326.  
 1 tps82 LI 1.00N 1.000 2.00 0.00 0.00 2 52.9465000 -368300.000  
 369.000 495.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12100.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.703274180D+04 -4.390844045D+01

LiNO2(L) Liquid. Gurvich,1982 pt1 p292 pt2 p326.  
 1 tps82 LI 1.00N 1.000 2.00 0.00 0.00 3 52.9465000 -368300.000  
 495.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12100.000  
 0.000000000D+00 0.000000000D+00 1.082445027D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.652158720D+04 -4.913541343D+01

## Appendix D (continued)

LiNO<sub>3</sub>(cr) Hexagonal. Gurvich,1982 pt1 p294 pt2 p328.  
 1 tps82 LI 1.00N 1.000 3.00 0.00 0.00 1 68.9459000 -482700.000  
 298.150 526.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12800.000  
 0.000000000D+00 0.000000000D+00 1.052906305D+01 -9.448181552D-03 3.365959028D-05  
 0.000000000D+00 0.000000000D+00 -6.107180100D+04 -4.616118415D+01

LiNO<sub>3</sub>(L) Liquid. Gurvich,1982 pt1 p294 pt2 p328.  
 1 tps82 LI 1.00N 1.000 3.00 0.00 0.00 2 68.9459000 -482700.000  
 525.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12800.000  
 0.000000000D+00 0.000000000D+00 1.792047878D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.162709200D+04 -8.706763908D+01

LiOH(cr) Tetragonal. Gurvich,1996b.  
 1 g 9/99 LI 1.00O 1.00H 1.00 0.00 0.00 1 23.9483400 -487500.000  
 200.000 746.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7414.000  
 -1.219596094D+06 2.088315832D+04 -1.463475951D+02 5.611592820D-01 -1.084380003D-03  
 1.071790003D-06 -4.218924790D-10 -1.553535026D+05 7.744131680D+02

LiOH(L) Liquid. Gurvich,1996b.  
 1 g 9/99 LI 1.00O 1.00H 1.00 0.00 0.00 2 23.9483400 -487500.000  
 746.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7414.000  
 0.000000000D+00 0.000000000D+00 1.049971676D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.050280710D+04 -5.407387960D+01

Li<sub>2</sub>CO<sub>3</sub>(cr) Monoclinic. Gurvich,1982 pt1 p297 pt2 p330.  
 2 tps82 LI 2.00C 1.000 3.00 0.00 0.00 1 73.8909000 -1214100.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15180.000  
 1.989594337D+07 -3.631706770D+05 2.691242782D+03 -1.033109020D+01 2.201400812D-02  
 -2.454585112D-05 1.122641035D-08 1.495415902D+06 -1.413251128D+04  
 500.000 1005.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15180.000  
 -5.276502280D+04 0.000000000D+00 7.025051540D+00 1.809479379D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.490977245D+05 -3.487871400D+01

Li<sub>2</sub>CO<sub>3</sub>(L) Liquid. Gurvich,1982 pt1 p297 pt2 p330.  
 1 tps82 LI 2.00C 1.000 3.00 0.00 0.00 2 73.8909000 -1214100.000  
 1005.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15180.000  
 0.000000000D+00 0.000000000D+00 2.225025888D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.502292112D+05 -1.169607936D+02

Li<sub>2</sub>O(cr) Cubic. Gurvich,1982 pt1 p257 pt2 p295.  
 2 tps82 LI 2.00O 1.00 0.00 0.00 0.00 1 29.8814000 -597880.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7251.000  
 3.028110639D+05 -4.262752720D+03 1.838105970D+01 8.164277890D-03 -6.056855750D-05  
 8.533995130D-08 -3.737236310D-11 -5.206402060D+04 -1.132207799D+02  
 800.000 1726.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7251.000  
 -5.016824310D+06 2.420062743D+04 -4.101266390D+01 5.324367340D-02 -2.998210001D-05  
 1.063865942D-08 -1.399118443D-12 -2.158188563D+05 2.784406390D+02

Li<sub>2</sub>O(L) Liquid. Gurvich,1982 pt1 p257 pt2 p295.  
 1 tps82 LI 2.00O 1.00 0.00 0.00 0.00 2 29.8814000 -597880.000  
 1726.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7251.000  
 0.000000000D+00 0.000000000D+00 1.250825364D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.338860760D+04 -6.881025076D+01

Li<sub>2</sub>O<sub>2</sub>(cr) Hexagonal. Gurvich,1982 pt1 p261 pt2 p298.  
 1 tps82 LI 2.00O 2.00 0.00 0.00 0.00 1 45.8808000 -632500.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10500.000  
 0.000000000D+00 0.000000000D+00 6.874488094D+00 7.197297255D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.844135590D+04 -3.433817812D+01

Li<sub>2</sub>SO<sub>4</sub>(a) Alpha. Gurvich,1982 pt1 p291 pt2 p325.  
 2 tps82 LI 2.00S 1.000 4.00 0.00 0.00 1 109.9446000 -1436000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18631.000  
 2.307314336D+07 -4.440850530D+05 3.473570360D+03 -1.406997202D+01 3.151077609D-02  
 -3.672532150D-05 1.742494307D-08 1.810572013D+06 -1.805254507D+04  
 500.000 848.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18631.000  
 1.379684430D+06 0.000000000D+00 -7.865353280D+01 4.280849920D-01 -6.782300830D-04  
 3.795553140D-07 0.000000000D+00 -1.584238676D+05 3.687429570D+02

Li<sub>2</sub>SO<sub>4</sub>(b) Beta. Gurvich,1982 pt1 p291 pt2 p325.  
 1 tps82 LI 2.00S 1.000 4.00 0.00 0.00 2 109.9446000 -1436000.000  
 848.000 1131.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18631.000  
 0.000000000D+00 0.000000000D+00 2.621922398D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.809832398D+05 -1.396630415D+02

Li<sub>2</sub>SO<sub>4</sub>(L) Liquid. Gurvich,1982 pt1 p291 pt2 p325.  
 1 tps82 LI 2.00S 1.000 4.00 0.00 0.00 3 109.9446000 -1436000.000  
 1131.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18631.000  
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.780963589D+05 -1.276811017D+02

## Appendix D (continued)

Li3ALF6(IV) Rhombic. Gurvich,1982 pt1 p301 pt2 p334.  
 2 tps82 LI 3.00AL 1.00F 6.00 0.00 0.00 1 161.7949572 -3389600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32150.000  
 -9.493305210D+05 1.726015181D+04-1.388395633D+02 7.441178510D-01-1.715868367D-03  
 2.058073373D-06-9.983283300D-10 -4.893133340D+05 7.043980840D+02  
 500.000 788.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32150.000  
 -3.361898910D+05 0.000000000D+00 2.259884943D+01 2.065859808D-02-6.977943650D-06  
 0.000000000D+00 0.000000000D+00 -4.163946960D+05-1.138999049D+02

Li3ALF6(III) Tetragonal. Gurvich,1982 pt1 p301 pt2 p334.  
 1 tps82 LI 3.00AL 1.00F 6.00 0.00 0.00 2 161.7949572 -3389600.000  
 788.000 873.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32150.000  
 0.000000000D+00 0.000000000D+00 3.427742585D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.195341580D+05-1.769490331D+02

Li3ALF6(II) Cubic. Gurvich,1982 pt1 p301 pt2 p334.  
 1 tps82 LI 3.00AL 1.00F 6.00 0.00 0.00 3 161.7949572 -3389600.000  
 873.000 978.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32150.000  
 0.000000000D+00 0.000000000D+00 3.548014255D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.202233150D+05-1.846804483D+02

Li3ALF6(I) Crystal. Gurvich,1982 pt1 p301 pt2 p334.  
 1 tps82 LI 3.00AL 1.00F 6.00 0.00 0.00 4 161.7949572 -3389600.000  
 978.000 1058.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32150.000  
 0.000000000D+00 0.000000000D+00 3.343552416D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.172975860D+05-1.696552845D+02

Li3ALF6(L) Liquid. Gurvich,1982 pt1 p301 pt2 p334.  
 1 tps82 LI 3.00AL 1.00F 6.00 0.00 0.00 5 161.7949572 -3389600.000  
 1058.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 32150.000  
 0.000000000D+00 0.000000000D+00 4.642486448D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.204684280D+05-2.501224871D+02

Li3N(cr) Chase,1998 p1526.  
 2 j 3/78 LI 3.00N 1.00 0.00 0.00 0.00 1 34.8297000 -164557.000  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11213.120  
 1.373485590D+06-2.379184204D+04 1.591917968D+02-4.823554940D-01 8.557283860D-04  
 -7.626448860D-07 2.741510774D-10 8.816502990D+04-8.595793090D+02  
 700.000 1300.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11213.120  
 -1.241718958D+08 7.830020910D+05-2.032330783D+03 2.815135927D+00-2.148359487D-03  
 8.689521850D-07-1.452735248D-10 -4.390747670D+06 1.278810396D+04

Mg(cr) Hexagonal. Ref-Elm. Alcock,1993.  
 2 srd 93 MG 1.00 0.00 0.00 0.00 0.00 1 24.3050000 0.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4979.161  
 -5.412225134D+03 0.000000000D+00 1.458173723D+00 1.330204666D-02-4.098858502D-05  
 4.754339101D-08 0.000000000D+00 -7.759472010D+02-6.989702348D+00  
 298.150 923.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4979.161  
 -2.860060304D+04 0.000000000D+00 3.398877384D+00-7.243962663D-04 1.405254188D-06  
 0.000000000D+00 0.000000000D+00 -1.089519906D+03-1.545973664D+01

Mg(L) Liquid. Ref-Elm. Alcock,1993.  
 1 srd 93 MG 1.00 0.00 0.00 0.00 0.00 2 24.3050000 0.000  
 923.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4979.161  
 0.000000000D+00 0.000000000D+00 4.125318269D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.589919480D+02-1.937828582D+01

MgAL2O4(cr) Crystal. Chase,1998 pp147-9.  
 2 j12/79 MG 1.00AL 2.000 4.00 0.00 0.00 1 142.2656760 -2299110.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 64479.624  
 9.746254450D+05-1.525021312D+04 8.302860630D+01-1.382241614D-01 1.657566530D-04  
 -9.668302460D-08 2.170561037D-11 -2.062543046D+05-4.734083400D+02  
 800.000 2408.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 64479.624  
 -7.339625410D+05 1.248275880D+03 1.548493786D+01 6.232746800D-03-9.669121680D-07  
 2.487422341D-10-2.603898110D-14 -2.909147610D+05-7.914855130D+01

MgAL2O4(L) Liquid. Chase,1998 pp147-9.  
 1 j12/79 MG 1.00AL 2.000 4.00 0.00 0.00 2 142.2656760 -2299110.000  
 2408.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 64479.624  
 0.000000000D+00 0.000000000D+00 2.641887495D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.688320250D+05-1.419843893D+02

MgBr2(cr) Hexagonal. Gurvich,1996a pt1 p418 pt2 p332.  
 1 tps96 MG 1.00BR 2.00 0.00 0.00 0.00 1 184.1130000 -526000.000  
 298.150 984.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15500.499  
 -6.657036915D+04 0.000000000D+00 9.124771033D+00 1.443260036D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.627087500D+04-3.872222733D+01

## Appendix D (continued)

MgBr2(L) Liquid. Gurvich,1996a pt1 p418 pt2 p332.  
 1 tps96 MG 1.00BR 2.00 0.00 0.00 0.00 2 184.1130000 -526000.000  
 984.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15500.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.363378060D+04-5.246637684D+01

MgCO3(cr) Hexagonal. Gurvich,1996a pt1 p429 pt2 p341.  
 2 tps96 MG 1.00C 1.000 3.00 0.00 0.00 1 84.3139000 -1096000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11630.499  
 -5.649471920D+06 1.059809340D+05-8.095953810D+02 3.267992680D+00-7.111639940D-03  
 8.088247340D-06-3.758639920D-09 -6.098528470D+05 4.221968000D+03  
 500.000 1263.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11630.499  
 -1.743337852D+05 0.000000000D+00 8.820122894D+00 7.696184141D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.353742560D+05-4.570039759D+01

MgCO3(L) Liquid. Gurvich,1996a pt1 p429 pt2 p341.  
 1 tps96 MG 1.00C 1.000 3.00 0.00 0.00 3 84.3139000 -1096000.000  
 1263.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11630.499  
 0.000000000D+00 0.000000000D+00 1.804075045D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.336474914D+05-9.615384273D+01

MgCL2(cr) Hexagonal. Gurvich,1996a pt1 p413 pt2 p329.  
 2 tps96 MG 1.00CL 2.00 0.00 0.00 0.00 1 95.2110000 -644300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13770.499  
 3.151271437D+05-4.986561670D+03 3.407490430D+01-6.013327030D-02 7.256223640D-05  
 -2.984411528D-08-5.064069590D-12 -5.608909370D+04-1.833415814D+02  
 500.000 987.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13770.499  
 -7.745495525D+04 0.000000000D+00 9.099153167D+00 1.199709905D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.051706960D+04-4.185795845D+01

MgCL2(L) Liquid. Gurvich,1996a pt1 p413 pt2 p329.  
 1 tps96 MG 1.00CL 2.00 0.00 0.00 0.00 3 95.2110000 -644300.000  
 987.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13770.499  
 7.120082843D+05 0.000000000D+00 1.060122605D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.543168500D+04-4.537295861D+01

MgF2(cr) Tetragonal. Gurvich,1996a pt1 p410 pt2 p326.  
 2 tps96 MG 1.00F 2.00 0.00 0.00 0.00 1 62.3018064 -1124200.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9920.499  
 -8.758857470D+06 1.630690293D+05-1.234784473D+03 4.913114430D+00-1.064398199D-02  
 1.204196054D-05-5.572295890D-09 -8.710379520D+05 6.452721700D+03  
 500.000 1536.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9920.499  
 -1.863609521D+05 0.000000000D+00 9.358338615D+00 4.871002621D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.386463039D+05-4.763420955D+01

MgF2(L) Liquid. Gurvich,1996a pt1 p410 pt2 p326.  
 1 tps96 MG 1.00F 2.00 0.00 0.00 0.00 3 62.3018064 -1124200.000  
 1536.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9920.499  
 0.000000000D+00 0.000000000D+00 1.140175428D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.340531621D+05-5.725828106D+01

MgH2(b) Beta,tetragonal. Gurvich,1996a pt1 p402 pt2 p321.  
 1 tps96 MG 1.00H 2.00 0.00 0.00 0.00 1 26.3208800 -75700.000  
 200.000 600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5310.000  
 4.034912200D+06-6.115400800D+04 3.537084270D+02-9.554057160D-01 1.260522797D-03  
 -6.389211330D-07 0.000000000D+00 2.799920215D+05-1.959491159D+03

MgH2(L) Liquid. Gurvich,1996a pt1 p402 pt2 p321.  
 1 tps96 MG 1.00H 2.00 0.00 0.00 0.00 2 26.3208800 -75700.000  
 600.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5310.000  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.135051728D+04-4.777194561D+01

MgI2(cr) Hexagonal. Gurvich,1996a pt1 p422 pt2 p335.  
 1 tps96 MG 1.00I 2.00 0.00 0.00 0.00 1 278.1139400 -370000.000  
 298.150 906.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17000.499  
 0.000000000D+00 0.000000000D+00 8.291528905D+00 2.232723275D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.707187430D+04-3.179107057D+01

MgI2(L) Liquid. Gurvich,1996a pt1 p422 pt2 p335.  
 1 tps96 MG 1.00I 2.00 0.00 0.00 0.00 2 278.1139400 -370000.000  
 906.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17000.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.641294920D+04-5.175282479D+01

## Appendix D (continued)

MgO(cr) Cubic Gurvich,1996a pt1 p397 pt2 p317.  
 2 tps96 MG 1.000 1.00 0.00 0.00 0.00 1 40.3044000 -601600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5160.499  
 -8.980784570D+05 1.771245421D+04-1.449325747D+02 6.397591100D-01-1.458346800D-03  
 1.715467374D-06-8.183482370D-10 -1.516290864D+05 7.439009690D+02  
 500.000 3100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5160.499  
 -1.169521716D+05 0.000000000D+00 5.510366817D+00 1.085932905D-03-4.866191754D-07  
 1.253230798D-10 0.000000000D+00 -7.443482720D+04-2.911564935D+01

MgO(L) Liquid Gurvich,1996a pt1 p397 pt2 p317.  
 1 tps96 MG 1.000 1.00 0.00 0.00 0.00 3 40.3044000 -601600.000  
 3100.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5160.499  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.609370840D+04-6.076894048D+01

Mg(OH)2(cr) Hexagonal. Gurvich,1996a pt1 p405 pt2 p323.  
 2 tps96 MG 1.000 2.00H 2.00 0.00 0.00 1 58.3196800 -924350.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11410.000  
 -6.401451840D+05 8.358139990D+03-3.971145400D+01 1.231927219D-01-9.647800650D-05  
 0.000000000D+00 0.000000000D+00 -1.537246903D+05 2.258495398D+02  
 500.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11410.000  
 -5.543828430D+06 3.700868610D+04-9.088623340D+01 1.431689186D-01-9.513965240D-05  
 2.532586546D-08 0.000000000D+00 -3.189450890D+05 5.801638270D+02

Mg(OH)2(L) Liquid. Gurvich,1996a pt1 p405 pt2 p323.  
 1 tps96 MG 1.000 2.00H 2.00 0.00 0.00 2 58.3196800 -924350.000  
 1100.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11410.000  
 -3.037581289D+05 0.000000000D+00 1.203462381D+01 2.202655358D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.158775486D+05-6.333852645D+01

MgS(cr) Cubic. Gurvich,1996a pt1 p424 pt2 p337.  
 2 tps96 MG 1.00S 1.00 0.00 0.00 0.00 1 56.3700000 -348000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8330.499  
 1.862529340D+06-3.536941040D+04 2.721839670D+02-1.042907730D+00 2.246733361D-03  
 -2.528313530D-06 1.164923631D-09 1.157121957D+05-1.421776433D+03  
 500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8330.499  
 -2.774667419D+04 0.000000000D+00 5.477652922D+00 1.053219011D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.362757840D+04-2.562621459D+01

MgS(L) Liquid. Gurvich,1996a pt1 p424 pt2 p337.  
 1 tps96 MG 1.00S 1.00 0.00 0.00 0.00 3 56.3700000 -348000.000  
 2500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8330.499  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.919942750D+04-4.015043492D+01

MgSO4(II) CrII,rhombic. Gurvich,1996a pt1 p426 pt2 p339.  
 2 tps96 MG 1.00S 1.000 4.00 0.00 0.00 1 120.3676000 -1288800.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15400.499  
 7.038799190D+06-1.283866938D+05 9.464955820D+02-3.562117130D+00 7.535844540D-03  
 -8.351428640D-06 3.800035070D-09 4.243566150D+05-4.979377480D+03  
 500.000 1283.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15400.499  
 -1.403690656D+05 0.000000000D+00 1.024474082D+01 1.053279147D-02-2.384385851D-06  
 0.000000000D+00 0.000000000D+00 -1.589785092D+05-5.117735953D+01

MgSO4(I) CrI,rhombic. Gurvich,1996a pt1 p426 pt2 p339.  
 1 tps96 MG 1.00S 1.000 4.00 0.00 0.00 3 120.3676000 -1288800.000  
 1283.000 1410.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15400.499  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.622917080D+05-9.940197517D+01

MgSO4(L) Liquid. Gurvich,1996a pt1 p426 pt2 p339.  
 1 tps96 MG 1.00S 1.000 4.00 0.00 0.00 4 120.3676000 -1288800.000  
 1410.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15400.499  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.605357417D+05-9.815660894D+01

MgSiO3(I) Chase,1998 pp1540-2.  
 1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 1 100.3887000 -1548916.800  
 200.000 903.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12112.680  
 6.634624630D+05-1.098828549D+04 6.661582640D+01-1.408979556D-01 2.056144180D-04  
 -1.506280668D-07 4.456006950D-11 -1.365977193D+05-3.704100780D+02

MgSiO3(II) Chase,1998 pp1540-2.  
 1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 2 100.3887000 -1548916.800  
 903.000 1258.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12112.680  
 0.000000000D+00 0.000000000D+00 1.447351774D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.916168640D+05-7.665690420D+01

## Appendix D (continued)

MgSiO<sub>3</sub>(III) Chase,1998 pp1540-2.  
 1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 3 100.3887000 -1548916.800  
 1258.000 1850.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12112.680  
 0.000000000D+00 0.000000000D+00 1.472512607D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.917371327D+05 -7.829669776D+01

MgSiO<sub>3</sub>(L) Chase,1998 pp1540-2.  
 1 j12/67 MG 1.00SI 1.000 3.00 0.00 0.00 4 100.3887000 -1548916.800  
 1850.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12112.680  
 0.000000000D+00 0.000000000D+00 1.761258330D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.880210286D+05 -9.512270574D+01

MgTiO<sub>3</sub>(cr) Chase,1998 pp1543-5.  
 2 j 6/67 MG 1.00TI 1.000 3.00 0.00 0.00 1 120.1702000 -1572556.400  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13556.160  
 7.429774000D+05 -1.292212821D+04 8.410507170D+01 -2.098263307D-01 3.615281930D-04  
 -3.238214780D-07 1.180955355D-10 -1.313766506D+05 -4.602729640D+02  
 700.000 1953.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13556.160  
 1.601922450D+05 -2.633226069D+03 1.883800780D+01 -1.678968165D-03 1.139243183D-06  
 -2.244954628D-10 2.663226969D-14 -1.791724552D+05 -1.059181291D+02

MgTiO<sub>3</sub>(L) Chase,1998 pp1543-5.  
 1 j 6/67 MG 1.00TI 1.000 3.00 0.00 0.00 2 120.1702000 -1572556.400  
 1953.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13556.160  
 0.000000000D+00 0.000000000D+00 1.962544997D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.909134805D+05 -1.065587855D+02

MgTi<sub>2</sub>O<sub>5</sub>(cr) Todd,1952. Chase,1998 pp1550-1552 6/67.  
 2 g11/00 MG 1.00TI 2.000 5.00 0.00 0.00 1 200.0360000 -2508218.800  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22438.792  
 1.244806767D+06 -2.122898938D+04 1.352816814D+02 -3.207171960D-01 5.056737150D-04  
 -4.075110600D-07 1.330675670D-10 -2.063427950D+05 -7.421883210D+02  
 800.000 1963.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22438.792  
 1.206826103D+06 -7.504042080D+03 3.472504430D+01 -9.398048060D-03 7.725115420D-06  
 -2.268307646D-09 2.728749772D-13 -2.651238294D+05 -1.981547532D+02

MgTi<sub>2</sub>O<sub>5</sub>(L) Todd,1952. Chase,1998 pp1550-1552 6/67.  
 1 g11/00 MG 1.00TI 2.000 5.00 0.00 0.00 2 200.0360000 -2508218.800  
 1963.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22438.792  
 0.000000000D+00 0.000000000D+00 3.140071995D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.039563022D+05 -1.685813857D+02

Mg<sub>2</sub>SiO<sub>4</sub>(cr) Chase,1998 pp1556-8 12/67.  
 2 g11/00 MG 2.00SI 1.000 4.00 0.00 0.00 1 140.6931000 -2177078.400  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17279.920  
 9.212035030D+05 -1.508156349D+04 9.085102220D+01 -1.898897815D-01 2.890690717D-04  
 -2.266693109D-07 7.230688250D-11 -1.936097830D+05 -5.059650070D+02  
 800.000 2171.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17279.920  
 3.714548590D+06 -2.041518891D+04 5.788009140D+01 -3.629874490D-02 2.183358474D-05  
 -6.504809080D-09 7.908133680D-13 -1.494870518D+05 -3.576608370D+02

Mg<sub>2</sub>SiO<sub>4</sub>(L) Chase,1998 pp1556-8 12/67  
 1 g11/00 MG 2.00SI 1.000 4.00 0.00 0.00 2 140.6931000 -2177078.400  
 2170.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17279.920  
 0.000000000D+00 0.000000000D+00 2.465761662D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.669357683D+05 -1.346103798D+02

Mg<sub>2</sub>TiO<sub>4</sub>(cr) Chase,1998 pp1559-61 6/67.  
 2 g11/00 MG 2.00TI 1.000 4.00 0.00 0.00 1 160.4746000 -2164354.400  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18836.368  
 9.956749990D+05 -1.724659186D+04 1.091877188D+02 -2.478088109D-01 3.830393010D-04  
 -3.022256428D-07 9.684735620D-11 -1.830794683D+05 -6.011710070D+02  
 800.000 2013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18836.368  
 3.251168130D+05 -3.023737890D+03 2.335313762D+01 -5.057540210D-04 2.750958409D-06  
 -9.172292550D-10 1.089453371D-13 -2.490728250D+05 -1.278129303D+02

Mg<sub>2</sub>TiO<sub>4</sub>(L) Chase,1998 pp1559-61 6/67.  
 1 g11/00 MG 2.00TI 1.000 4.00 0.00 0.00 2 160.4746000 -2164354.400  
 2013.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18836.368  
 0.000000000D+00 0.000000000D+00 2.747562995D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.615257868D+05 -1.474539637D+02

Mg<sub>3</sub>N<sub>2</sub>(cr) Cubic. Gurvich,1996a pt1 p427 pt2 p340.  
 1 tpis96 MG 3.00N 2.00 0.00 0.00 0.00 1 100.9284000 -461300.000  
 298.150 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10500.499  
 -3.313123684D+05 0.000000000D+00 1.448912804D+01 1.035659347D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.095851350D+04 -7.450243529D+01

## Appendix D (continued)

Mn(a) Alpha. Ref-Elm. Chase,1998 pp1571-4.  
 1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 1 54.9380490 0.000  
 200.000 980.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4994.000  
 -1.984724642D+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 pp1571-4.  
 1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 2 54.9380490 0.000  
 980.000 1361.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4994.000  
 -2.033299729D+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 pp1571-4.  
 1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 3 54.9380490 0.000  
 1361.000 1412.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4994.000  
 -5.539443490D+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 pp1571-4.  
 1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 4 54.9380490 0.000  
 1412.000 1519.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4994.000  
 -4.256613510D+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 pp1571-4.  
 1 j 9/67 MN 1.00 0.00 0.00 0.00 0.00 5 54.9380490 0.000  
 1519.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4994.000  
 0.000000000D+00 0.000000000D+00 5.535383324D+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 pp1577-80.  
 3 j 3/78 MO 1.00 0.00 0.00 0.00 0.00 1 95.9400000 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4585.000  
 -4.961689320D+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 pp1577-80.  
 1 j 3/78 MO 1.00 0.00 0.00 0.00 0.00 2 95.9400000 0.000  
 2896.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4585.000  
 0.000000000D+00 0.000000000D+00 4.528949992D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 2.022300696D+03-2.280790783D+01

MoO2(cr) Monoclinic. Gurvich,1982 pt1 p27 pt2 p32.  
 2 tpis82 MO 1.000 2.00 0.00 0.00 0.00 1 127.9388000 -589300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8328.000  
 -6.526622370D+06 1.230156278D+05-9.443937510D+02 3.807393330D+00-8.319729080D-03  
 9.477106540D-06-4.408972390D-09 -6.244588120D+05 4.921849140D+03  
 500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8328.000  
 -2.051418601D+05 0.000000000D+00 8.963295880D+00-1.128973209D-04 1.146693959D-06  
 0.000000000D+00 0.000000000D+00 -7.424162440D+04-4.664669130D+01

MoO3(cr) Rhombic. Gurvich,1982 pt1 p30 pt2 p34.  
 2 tpis82 MO 1.000 3.00 0.00 0.00 0.00 1 143.9382000 -744600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12590.000  
 9.061545810D+06-1.658675979D+05 1.230236799D+03-4.691503730D+00 9.965828580D-03  
 -1.109194136D-05 5.065628490D-09 6.590937470D+05-6.461598540D+03  
 500.000 1075.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12590.000  
 -9.462974968D+04 0.000000000D+00 8.841771794D+00 4.197842086D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.269445280D+04-4.282025959D+01

MoO3(L) Liquid. Gurvich,1982 pt1 p30 pt2 p34.  
 1 tpis82 MO 1.000 3.00 0.00 0.00 0.00 3 143.9382000 -744600.000  
 1075.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12590.000  
 0.000000000D+00 0.000000000D+00 1.527450205D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.123881420D+04-7.771899557D+01

NH4CL(II) Chase,1998 p765.  
 1 j 9/65 N 1.00H 4.00CL 1.00 0.00 0.00 1 53.4914600 -314553.000  
 298.150 457.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22698.000  
 1.593389657D+05 0.000000000D+00-5.965854940D+00 6.494193170D-02-5.391456890D-05  
 0.000000000D+00 0.000000000D+00 -3.792881500D+04 2.933013040D+01

## Appendix D (continued)

NH<sub>4</sub>CL(III) Chase,1998 p765.

2 j 9/65 N	1.00H	4.00CL	1.00	0.00	0.00	2	53.4914600	-314553.000
457.700	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.641820157D+07	1.639262758D+05	-6.654529630D+02	1.447086973D+00	-1.698254160D-03				
1.056255415D-06	-2.697574651D-10		-8.787975900D+05	3.897936900D+03				
1000.000	1500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
8.409592660D+08	-3.426760780D+06	5.548091470D+03	-4.435674300D+00	1.772486202D-03				
-2.817160120D-07	0.000000000D+00		2.063363145D+07	-3.765976360D+04				

NH<sub>4</sub>F(cr) Hexagonal. Gurvich,1989 pt1 p388 pt2 p324.

2 tpis89 N	1.00H	4.00F	1.00	0.00	0.00	1	37.0368632	-467560.000
200.000	298.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-2.975636383D+06	7.208754230D+04	-7.346289470D+02	4.075299810D+00	-1.264044498D-02				
2.111837237D-05	-1.479873524D-08		-3.621184440D+05	3.608760970D+03				
298.150	511.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.563531705D+00	2.108482641D-02	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-5.763754000D+04	-6.538862038D+00				

NH<sub>4</sub>F(L) Liquid. Gurvich,1989 pt1 p388 pt2 p324.

1 tpis89 N	1.00H	4.00F	1.00	0.00	0.00	2	37.0368632	-467560.000
511.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.359069867D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-5.951515380D+04	-6.780477125D+01				

Na(cr) Cubic. Ref-Elm. Cox,1989 p254.

1 coda89 NA	1.00	0.00	0.00	0.00	0.00	1	22.9897700	0.000
200.000	371.0107	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-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	22.9897700	0.000
371.010	2300.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
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				

NaAlO<sub>2</sub>(a) Alpha. Chase,1998 p131.

1 j 3/63 NA	1.00AL	1.000	2.00	0.00	0.00	1	81.9701080	-1133190.000
200.000	740.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.527204140D+05	-7.722924360D+03	5.000166380D+01	-1.091293529D-01	1.762084005D-04				
-1.452865027D-07	4.918123650D-11		-1.021205450D+05	-2.738871707D+02				

NaAlO<sub>2</sub>(b) Beta. Chase,1998 p131.

1 j 3/63 NA	1.00AL	1.000	2.00	0.00	0.00	2	81.9701080	-1133190.000
740.000	3000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.197980170D+06	-1.525937524D+04	3.932924030D+01	-2.623291355D-02	1.465112353D-05				
-3.740532770D-09	3.560249390D-13		-4.988553210D+04	-2.434131708D+02				

NaBO<sub>2</sub>(cr) Hexagonal. Gurvich,1982 pt1 p357 pt2 p391.

2 tpis82 NA	1.00B	1.000	2.00	0.00	0.00	1	65.7995700	-976500.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.074702306D+05	2.343688910D+03	-1.964636192D+01	1.319434021D-01	-2.997058540D-04				
3.640103610D-07	-1.796104124D-10		-1.291527393D+05	9.915788280D+01				
500.000	1239.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.597627870D+04	0.000000000D+00	5.491743560D+00	1.171509302D-02	-4.773472260D-06				
0.000000000D+00	0.000000000D+00		-1.197489098D+05	-2.604168849D+01				

NaBO<sub>2</sub>(L) Liquid. Gurvich,1982 pt1 p357 pt2 p391.

1 tpis82 NA	1.00B	1.000	2.00	0.00	0.00	2	65.7995700	-976500.000
1239.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.743939210D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.245121293D+05	-9.701235601D+01				

NaBr(cr) Cubic. Gurvich,1982 pt1 p340 pt2 p378.

2 tpis82 NA	1.00BR	1.00	0.00	0.00	0.00	1	102.8937700	-361160.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
3.210289070D+06	-5.986721400D+04	4.572531830D+02	-1.768432397D+00	3.814169490D-03				
-4.295102010D-06	1.980139146D-09		2.245558598D+05	-2.385763453D+03				
500.000	1020.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.593247644D+04	0.000000000D+00	5.272913580D+00	2.440774360D-03	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-4.506450850D+04	-2.022580453D+01				

NaBr(L) Liquid. Gurvich,1982 pt1 p340 pt2 p378.

1 tpis82 NA	1.00BR	1.00	0.00	0.00	0.00	2	102.8937700	-361160.000
1020.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	8.178473536D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-4.361938300D+04	-3.477943790D+01				



## Appendix D (continued)

NaCN(II)                      Lambda trans@288.5K. Chase,1998(3/66) pp631-3. Messer,1941.

6 g 8/01 NA	1.00C	1.00N	1.00	0.00	0.00	1	49.0071700	-90709.000
197.700	245.9007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
4.995073610D+08	-1.007656780D+07	7.458386410D+04	-2.134406974D+02	-6.965856220D-02				
1.540182072D-03	-2.204709373D-06		4.493712560D+07	-3.984423000D+05				
245.900	273.1007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.546907220D+08	4.339535660D+06	5.476070770D+02	-1.324240852D+02	5.045446840D-01				
-5.791737950D-04	0.000000000D+00		-2.385188911D+07	3.106410058D+04				
273.100	284.2007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-4.415096320D+08	0.000000000D+00	3.452631670D+04	-1.661761169D+02	2.250608921D-01				
0.000000000D+00	0.000000000D+00		-6.388306670D+06	-1.596447272D+05				
284.200	286.3007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.647379186D+09	0.000000000D+00	-6.100370390D+04	1.429224260D+02	0.000000000D+00				
0.000000000D+00	0.000000000D+00		1.735057318D+07	3.142435378D+05				
286.300	287.7007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.607424258D+11	0.000000000D+00	-8.629992400D+06	3.290155880D+04	-3.355904228D+01				
0.000000000D+00	0.000000000D+00		1.946284579D+09	4.175641230D+07				
287.700	288.5007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.494237648D+11	0.000000000D+00	8.652205900D+06	-3.521604880D+04	3.968501633D+01				
0.000000000D+00	0.000000000D+00		-1.866195945D+09	-4.140143280D+07				

NaCN(III)                      Lambda trans@288.5K. Chase,1998(3/66) pp631-3. Messer,1941.

3 g 8/01 NA	1.00C	1.00N	1.00	0.00	0.00	2	49.0071700	-90709.000
288.500	290.4007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	5.590153690D+06	-4.787600130D+04	1.309325625D+02				
-1.114230434D-01	0.000000000D+00		-4.753893060D+08	-2.241133349D+07				
290.400	293.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	1.752406137D+07	-1.788423367D+05	6.083847560D+02				
-6.898560518D-01	0.000000000D+00		-1.287828620D+09	-6.746932890D+07				
293.150	835.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	8.303074986D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.338528469D+04	-3.306050253D+01				

NaCN(L)                      Chase,1998(3/66) pp631-3. Messer,1941.

1 g 8/01 NA	1.00C	1.00N	1.00	0.00	0.00	3	49.0071700	-90709.000
835.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	9.561116650D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.337899448D+04	-4.025831708D+01				

NaCl(cr)                      Cubic. Gurvich,1982 pt1 p335 pt2 p374.

2 tps82 NA	1.00CL	1.00	0.00	0.00	0.00	1	58.4427700	-411260.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.725695501D+06	-5.160958750D+04	3.984582310D+02	-1.547496756D+00	3.352172310D-03				
-3.787781590D-06	1.751729541D-09		1.807530763D+05	-2.076949046D+03				
500.000	1074.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
2.657827371D+03	0.000000000D+00	5.665718690D+00	8.708901490D-04	1.340560030D-06				
0.000000000D+00	0.000000000D+00		-5.119384720D+04	-2.390773149D+01				

NaCl(L)                      Liquid. Gurvich,1982 pt1 p335 pt2 p374.

1 tps82 NA	1.00CL	1.00	0.00	0.00	0.00	2	58.4427700	-411260.000
1074.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	8.166446369D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-4.943459010D+04	-3.649536621D+01				

NaF(cr)                      Cubic. Gurvich,1982 pt1 p330 pt2 p370.

2 tps82 NA	1.00F	1.00	0.00	0.00	0.00	1	41.9881732	-576600.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-6.479380410D+06	1.203694117D+05	-9.069923560D+02	3.596486550D+00	-7.775987760D-03				
8.784072120D-06	-4.059177020D-09		-6.130723750D+05	4.744846560D+03				
500.000	1269.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.103659993D+05	0.000000000D+00	7.264294880D+00	-1.973449856D-03	2.198504269D-06				
0.000000000D+00	0.000000000D+00		-7.181627510D+04	-3.536594020D+01				

NaF(L)                      Liquid. Gurvich,1982 pt1 p330 pt2 p370.

1 tps82 NA	1.00F	1.00	0.00	0.00	0.00	2	41.9881732	-576600.000
1269.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	8.431044042D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-6.918200450D+04	-4.115725624D+01				

NaH(cr)                      Cubic. Gurvich,1982 pt1 p324 pt2 p365.

2 tps82 NA	1.00H	1.00	0.00	0.00	0.00	1	23.9977100	-56380.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-7.991749220D+05	1.540118135D+04	-1.207582590D+02	5.162361030D-01	-1.142424910D-03				
1.321529809D-06	-6.221705120D-10		-7.637675350D+04	6.264186650D+02				
500.000	911.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-5.921209820D+04	0.000000000D+00	3.776579530D+00	4.250132020D-03	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-8.294394750D+03	-1.830678857D+01				

## Appendix D (continued)

NaH(L) Liquid. Gurvich,1982 pt1 p324 pt2 p365.  
 1 tps82 NA 1.00H 1.00 0.00 0.00 0.00 2 23.9977100 -56380.000  
 911.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6259.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.034013160D+03-3.112842170D+01

NaI(cr) Cubic. Gurvich,1982 pt1 p343 pt2 p381.  
 2 tps82 NA 1.00I 1.00 0.00 0.00 0.00 1 149.8942400 -289630.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12260.000  
 3.500848300D+06-6.540492260D+04 5.005676630D+02-1.943541204D+00 4.201134090D-03  
 -4.738515580D-06 2.187428593D-09 2.579135069D+05-2.609575154D+03  
 500.000 934.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12260.000  
 2.799960757D+04 0.000000000D+00 5.047026160D+00 3.029892968D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.637984440D+04-1.764780816D+01

NaI(L) Liquid. Gurvich,1982 pt1 p343 pt2 p381.  
 1 tps82 NA 1.00I 1.00 0.00 0.00 0.00 2 149.8942400 -289630.000  
 934.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12260.000  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.505265490D+04-3.237951568D+01

NaNO2(I) Rhombic. Gurvich,1982 pt1 p350 pt2 p386.  
 2 tps82 NA 1.00N 1.000 2.00 0.00 0.00 1 68.9952700 -354600.000  
 298.150 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16500.000  
 1.090298767D+06 0.000000000D+00-3.023894373D+01 8.811824148D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.389227900D+04 1.648982675D+02  
 400.000 436.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16500.000  
 0.000000000D+00 0.000000000D+00 5.419446245D+02-1.998525469D+00 0.000000000D+00  
 4.207630035D-06 0.000000000D+00 -1.254887886D+05-2.521831769D+03

NaNO2(I') Rhombic. Gurvich,1982 pt1 p350 pt2 p386.  
 1 tps82 NA 1.00N 1.000 2.00 0.00 0.00 2 68.9952700 -354600.000  
 436.700 557.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16500.000  
 0.000000000D+00 0.000000000D+00 1.599613206D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.773155280D+04-7.952982535D+01

NaNO2(L) Liquid. Gurvich,1982 pt1 p350 pt2 p386.  
 1 tps82 NA 1.00N 1.000 2.00 0.00 0.00 3 68.9952700 -354600.000  
 557.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16500.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.372398050D+04-5.120982634D+01

NaNO3(a) Hexagonal. Gurvich,1982 pt1 p353 pt2 p388.  
 2 tps82 NA 1.00N 1.000 3.00 0.00 0.00 1 84.9946700 -467700.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17230.000  
 -4.851300240D+07 9.186316330D+05-7.046384650D+03 2.807834358D+01-6.098595830D-02  
 6.858389720D-05-3.110743577D-08 -4.182115940D+06 3.676430560D+04  
 500.000 549.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17230.000  
 0.000000000D+00 0.000000000D+00 2.680735245D+01-1.753272291D-01 3.165502236D-04  
 0.000000000D+00 0.000000000D+00 -5.811076460D+04-9.741742276D+01

NaNO3(b) Hexagonal. Gurvich,1982 pt1 p353 pt2 p388.  
 1 tps82 NA 1.00N 1.000 3.00 0.00 0.00 2 84.9946700 -467700.000  
 549.000 579.6007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17230.000  
 0.000000000D+00 0.000000000D+00 1.683803375D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.159974430D+04-8.308035085D+01

NaNO3(L) Liquid. Gurvich,1982 pt1 p353 pt2 p388.  
 1 tps82 NA 1.00N 1.000 3.00 0.00 0.00 3 84.9946700 -467700.000  
 579.600 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17230.000  
 0.000000000D+00 0.000000000D+00 1.695830542D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.985936520D+04-8.072256364D+01

NaOH(a) Alpha. Gurvich,1996b.  
 2 g 5/99 NA 1.00O 1.00H 1.00 0.00 0.00 1 39.9971100 -425800.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10490.000  
 2.008329119D+04-7.714677160D+02 8.694171090D+00 3.850883340D-03-3.610498540D-06  
 0.000000000D+00 0.000000000D+00 -4.948023450D+04-4.524899570D+01  
 298.150 514.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10490.000  
 1.048215710D+06 0.000000000D+00-9.592892425D+01 6.189564989D-01-1.367212259D-03  
 1.067453163D-06 0.000000000D+00 -3.663541040D+04 4.270051072D+02

NaOH(b) Beta. Gurvich,1996b.  
 1 g 5/99 NA 1.00O 1.00H 1.00 0.00 0.00 2 39.9971100 -425800.000  
 514.000 568.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10490.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.442558950D+04-4.799292559D+01

## Appendix D (continued)

NaOH(c)                    Gamma. Gurvich,1996b.  
 1 g 5/99 NA 1.000 1.00H 1.00 0.00 0.00 3 39.9971100 -425800.000  
 568.000 594.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10490.000  
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.407054750D+04 -5.122288687D+01

NaOH(L)                    Liquid. Gurvich,1996b.  
 2 g 5/99 NA 1.000 1.00H 1.00 0.00 0.00 4 39.9971100 -425800.000  
 594.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10490.000  
 0.000000000D+00 0.000000000D+00 1.077790513D+01 -7.111663826D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.343827480D+04 -5.228806116D+01  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10490.000  
 0.000000000D+00 0.000000000D+00 1.006673875D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.308269160D+04 -4.808666421D+01

Na2O(cr)                   Cubic. Gurvich,1982 pt1 p319 pt2 p359. Chase,1998 p1646 6/63.  
 1 g10/99 NA 1.000 2.00 0.00 0.00 0.00 1 54.9885700 -261000.000  
 223.300 825.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18300.000  
 0.000000000D+00 0.000000000D+00 7.541274230D+00 3.803351009D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.380838310D+04 -3.016162188D+01

Na2O(L)                   Liq. Gurvich,1982 pt1 p319 pt2 p359. Chase,1998 p1646 6/63.  
 1 g10/99 NA 1.000 2.00 0.00 0.00 0.00 2 54.9885700 -261000.000  
 825.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18300.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.374934750D+04 -5.415977808D+01

Na2CO3(a)                  Alpha,monoclinic. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tps82 NA 2.00C 1.000 3.00 0.00 0.00 1 105.9884400 -1129190.000  
 200.000 623.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20750.000  
 -2.240230091D+06 3.426046630D+04 -2.061520520D+02 7.168720430D-01 -1.253560327D-03  
 1.178136083D-06 -4.526962410D-10 -2.999635262D+05 1.125584713D+03

Na2CO3(b)                  Beta,monoclinic. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tps82 NA 2.00C 1.000 3.00 0.00 0.00 2 105.9884400 -1129190.000  
 623.000 752.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20750.000  
 0.000000000D+00 0.000000000D+00 7.711578914D+00 1.943638290D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.388766027D+05 -3.334178005D+01

Na2CO3(c)                  Gamma,hexagonal. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tps82 NA 2.00C 1.000 3.00 0.00 0.00 3 105.9884400 -1129190.000  
 752.000 1131.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20750.000  
 0.000000000D+00 0.000000000D+00 4.430327223D+00 1.645316441D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.353130199D+05 -9.031669943D+00

Na2CO3(L)                  Liquid. Gurvich,1982 pt1 p356 pt2 p390.  
 1 tps82 NA 2.00C 1.000 3.00 0.00 0.00 4 105.9884400 -1129190.000  
 1131.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20750.000  
 0.000000000D+00 0.000000000D+00 2.345297558D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.429369053D+05 -1.211911225D+02

Na2O(c)                    Gamma. Gurvich,1982 pt1 p320 pt2 p360.  
 2 tps82 NA 2.000 1.00 0.00 0.00 0.00 1 61.9789400 -414570.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12400.000  
 1.662637910D+06 -3.189091340D+04 2.474349303D+02 -9.313593580D-01 2.006501256D-03  
 -2.253952071D-06 1.037067374D-09 9.127774380D+04 -1.292003778D+03  
 500.000 1023.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12400.000  
 2.551096288D+05 -2.539111311D+03 1.659817003D+01 -1.233767744D-02 1.540713549D-05  
 -8.084697830D-09 1.747972425D-12 -3.906526610D+04 -8.958024740D+01

Na2O(b)                    Beta. Gurvich,1982 pt1 p320 pt2 p360.  
 1 tps82 NA 2.000 1.00 0.00 0.00 0.00 2 61.9789400 -414570.000  
 1023.000 1243.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12400.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.485897470D+04 -6.235394464D+01

Na2O(a)                    Alpha. Gurvich,1982 pt1 p320 pt2 p360.  
 1 tps82 NA 2.000 1.00 0.00 0.00 0.00 3 61.9789400 -414570.000  
 1243.000 1405.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12400.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.377652960D+04 -6.148311196D+01

Na2O(L)                    Liquid. Gurvich,1982 pt1 p320 pt2 p360.  
 1 tps82 NA 2.000 1.00 0.00 0.00 0.00 4 61.9789400 -414570.000  
 1405.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12400.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.944674950D+04 -5.840141793D+01

## Appendix D (continued)

Na2O2 (b)                   Beta. Gurvich,1982 pt1 p323 pt2 p363.

2 tps82 NA	2.000	2.00	0.00	0.00	0.00	1	77.9783400	-512000.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15694.000

-8.122024280D+05 1.451270156D+04-1.058114918D+02 4.802903390D-01-1.057140356D-03  
1.219343411D-06-5.728124010D-10 -1.295899700D+05 5.525239130D+02  
500.000 785.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15694.000  
-1.051839392D+05 0.000000000D+00 1.054275850D+01 4.638430480D-03 4.381769570D-09  
0.000000000D+00 0.000000000D+00 -6.528135100D+04-5.064487560D+01

Na2O2 (a)                   Alpha. Gurvich,1982 pt1 p323 pt2 p363.

1 tps82 NA	2.000	2.00	0.00	0.00	0.00	2	77.9783400	-512000.000
785.000	948.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15694.000

0.000000000D+00 0.000000000D+00 1.359069867D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.546547070D+04-6.641239933D+01

Na2O2 (L)                   Liquid. Gurvich,1982 pt1 p323 pt2 p363.

1 tps82 NA	2.000	2.00	0.00	0.00	0.00	3	77.9783400	-512000.000
948.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								15694.000

0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -6.581522070D+04-8.156770675D+01

Na2S (cr)                   Below lambda trans. Chase,1998 pp1667-9.

2 j 3/78 NA	2.00S	1.00	0.00	0.00	0.00	1	78.0445400	-366100.000
298.150	700.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								0.000

-4.541358110D+05 4.959201300D+03-1.171687783D+01 4.586680300D-02-4.501505030D-05  
1.801159260D-08 0.000000000D+00 -7.199330320D+04 8.057734670D+01  
700.000 1276.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
-3.527498880D+09 2.408466098D+07-6.783369110D+04 1.008062531D+02-8.320894540D-02  
3.611294520D-05-6.422558180D-09 -1.325119033D+08 4.212898800D+05

Na2S (cr)                   Above lambda trans. Chase,1998 pp1667-9.

1 j 3/78 NA	2.00S	1.00	0.00	0.00	0.00	2	78.0445400	-366100.000
1276.000	1445.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								0.000

8.868348820D+08 0.000000000D+00-2.045962174D+03 1.675387705D+00-3.752802310D-04  
0.000000000D+00 0.000000000D+00 2.169500522D+06 1.309983113D+04

Na2S (L)                   Chase,1998 pp1667-9.

1 j 3/78 NA	2.00S	1.00	0.00	0.00	0.00	3	78.0445400	-366100.000
1445.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								0.000

0.000000000D+00 0.000000000D+00 1.107076665D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -4.262953690D+04-4.848427350D+01

Na2SO3 (cr)                   Crystal. Barin,1989 pt2 p1002.

1 bar 89 NA	2.00S	1.000	3.00	0.00	0.00	1	126.0427400	-1100802.000
298.150	1184.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								0.000

0.000000000D+00 0.000000000D+00 1.290193602D+01 5.233511440D-03 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.364746191D+05-5.751819280D+01

Na2SO3 (L)                   Liquid. Barin,1989 pt2 p1002.

1 bar 89 NA	2.00S	1.000	3.00	0.00	0.00	2	126.0427400	-1100802.000
1184.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								0.000

0.000000000D+00 0.000000000D+00 2.188992496D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.403382187D+05-1.123000267D+02

Na2SO4 (V)                   Rhombic. Gurvich,1982 pt1 p346 pt2 p384.

1 tps82 NA	2.00S	1.000	4.00	0.00	0.00	1	142.0421400	-1387900.000
200.000	458.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								23204.000

-8.689043820D+05 1.449012038D+04-9.087576950D+01 3.621919930D-01-5.592870850D-04  
3.463421130D-07 0.000000000D+00 -2.371450313D+05 4.932876470D+02

Na2SO4 (IV)                   Rhombic. Gurvich,1982 pt1 p346 pt2 p384.

1 tps82 NA	2.00S	1.000	4.00	0.00	0.00	2	142.0421400	-1387900.000
458.000	514.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								23204.000

-1.455046659D+05 0.000000000D+00 1.308904554D+01 1.323950539D-02 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.718682018D+05-6.127355231D+01

Na2SO4 (I)                   Hexagonal. Gurvich,1982 pt1 p346 pt2 p384.

1 tps82 NA	2.00S	1.000	4.00	0.00	0.00	3	142.0421400	-1387900.000
514.000	1157.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								23204.000

0.000000000D+00 0.000000000D+00 2.503069934D+01-1.581223668D-02 1.591831629D-05  
0.000000000D+00 0.000000000D+00 -1.732950425D+05-1.201603231D+02

Na2SO4 (L)                   Liquid. Gurvich,1982 pt1 p346 pt2 p384.

1 tps82 NA	2.00S	1.000	4.00	0.00	0.00	4	142.0421400	-1387900.000
1157.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.0								23204.000

0.000000000D+00 0.000000000D+00 2.453542061D+01 0.000000000D+00 0.000000000D+00  
0.000000000D+00 0.000000000D+00 -1.722609524D+05-1.218642150D+02

## Appendix D (continued)

Na3ALF6(a) Monoclinic. Gurvich,1982 pt1 p361 pt2 p394.  
 2 tps82 NA 3.00AL 1.00F 6.00 0.00 0.00 1 209.9412672 -3322400.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38070.000  
 1.564580425D+07-2.923454204D+05 2.211217567D+03-8.502636700D+00 1.825363780D-02  
 -2.047448239D-05 9.409455420D-09 9.119433290D+05-1.157646461D+04  
 500.000 838.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38070.000  
 -1.416702978D+05 0.000000000D+00 2.315158739D+01 1.479360403D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.076260850D+05-1.084672805D+02

Na3ALF6(b) Cubic. Gurvich,1982 pt1 p361 pt2 p394.  
 1 tps82 NA 3.00AL 1.00F 6.00 0.00 0.00 2 209.9412672 -3322400.000  
 838.000 1286.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38070.000  
 0.000000000D+00 0.000000000D+00 2.624279723D+01 7.980987454D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.065549160D+05-1.221511986D+02

Na3ALF6(L) Liquid. Gurvich,1982 pt1 p361 pt2 p394.  
 1 tps82 NA 3.00AL 1.00F 6.00 0.00 0.00 3 209.9412672 -3322400.000  
 1286.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38070.000  
 0.000000000D+00 0.000000000D+00 4.702622283D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.129238590D+05-2.499831311D+02

Na5AL3F14(cr) Tetragonal. Gurvich,1982 pt1 p362 pt2 p395.  
 2 tps82 NA 5.00AL 3.00F 14.00 0.00 0.00 1 461.8711088 -7555000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 80830.000  
 -2.302157125D+07 4.240174110D+05-3.188373880D+03 1.288416515D+01-2.796179544D-02  
 3.169729270D-05-1.469118702D-08 -2.832459181D+06 1.667109223D+04  
 500.000 1010.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 80830.000  
 -8.720901540D+05 0.000000000D+00 6.109021050D+01 1.113784152D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.302863450D+05-2.943295261D+02

Na5AL3F14(L) Liquid. Gurvich,1982 pt1 p362 pt2 p395.  
 1 tps82 NA 5.00AL 3.00F 14.00 0.00 0.00 2 461.8711088 -7555000.000  
 1010.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 80830.000  
 0.000000000D+00 0.000000000D+00 1.171446062D+02 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.528147600D+05-6.431511436D+02

Nb(cr) Crystal. Ref-Elm. Chase,1998 pp1675-8.  
 3 j12/73 NB 1.00 0.00 0.00 0.00 0.00 1 92.9063800 0.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5241.000  
 -4.254811710D+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 pp1675-8.  
 1 j12/73 NB 1.00 0.00 0.00 0.00 0.00 2 92.9063800 0.000  
 2750.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5241.000  
 0.000000000D+00 0.000000000D+00 4.025733326D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 1.427029683D+03-1.857965621D+01

NbO(cr) Cubic. Gurvich,1982 pt1 p75 pt2 p77.  
 1 tps82 NB 1.000 1.00 0.00 0.00 0.00 1 108.9057800 -406000.000  
 298.150 2217.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7200.000  
 -4.430808310D+04 0.000000000D+00 5.073540112D+00 1.194297680D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.054466650D+04-2.397978879D+01

NbO(L) Liquid. Gurvich,1982 pt1 p75 pt2 p77.  
 1 tps82 NB 1.000 1.00 0.00 0.00 0.00 2 108.9057800 -406000.000  
 2217.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7200.000  
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.765976820D+04-3.975547844D+01

NbOCL3(cr) Barin,1989 pt2 p1030. Wagman,1982 p207.  
 1 bar 89 NB 1.000 1.00CL 3.00 0.00 0.00 1 215.2647800 -879500.000  
 298.150 702.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -1.822304138D+05 4.828593360D+02 1.341861113D+01 7.546458250D-03-1.198129404D-05  
 9.997155720D-09-3.425554610D-12 -1.133897355D+05-6.057973360D+01

NbO2(II) Tetragonal. Gurvich,1982 pt1 p78 pt2 p80.  
 2 tps82 NB 1.000 2.00 0.00 0.00 0.00 1 124.9051800 -795000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9267.000  
 -3.914505940D+06 7.500739880D+04-5.854724840D+02 2.416380822D+00-5.358130280D-03  
 6.172498470D-06-2.893870224D-09 -4.324424750D+05 3.040766836D+03  
 500.000 1082.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9267.000  
 -2.074227934D+05 0.000000000D+00 1.075172627D+01-7.363421090D-03 7.988904160D-06  
 0.000000000D+00 0.000000000D+00 -9.926049480D+04-5.405566340D+01

## Appendix D (continued)

NbO<sub>2</sub>(I) Tetragonal. Gurvich,1982 pt1 p78 pt2 p80.  
 1 tps82 NB 1.000 2.00 0.00 0.00 0.00 2 124.9051800 -795000.000  
 1082.000 2360.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9267.000  
 -2.470500366D+05 0.000000000D+00 1.027937906D+01 1.610437657D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.951665200D+04-5.395968051D+01

NbO<sub>2</sub>(L) Liquid. Gurvich,1982 pt1 p78 pt2 p80.  
 1 tps82 NB 1.000 2.00 0.00 0.00 0.00 3 124.9051800 -795000.000  
 2360.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9267.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.406789930D+04-6.330929540D+01

Nb<sub>2</sub>O<sub>5</sub>(cr) Monoclinic. Gurvich,1982 pt1 p81 pt2 p82.  
 2 tps82 NB 2.000 5.00 0.00 0.00 0.00 1 265.8097600 -1897000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22240.000  
 2.640209200D+07-4.944721050D+05 3.755171780D+03-1.472158158D+01 3.190561080D-02  
 -3.609939830D-05 1.669960716D-08 1.993996743D+06-1.963185769D+04  
 500.000 1783.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22240.000  
 2.666894830D+05 0.000000000D+00-3.157808421D+00 7.820838380D-02-9.622327490D-05  
 5.100828450D-08-9.357603760D-12 -2.290426814D+05 1.650612260D+01

Nb<sub>2</sub>O<sub>5</sub>(L) Liquid. Gurvich,1982 pt1 p81 pt2 p82.  
 1 tps82 NB 2.000 5.00 0.00 0.00 0.00 2 265.8097600 -1897000.000  
 1783.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22240.000  
 0.000000000D+00 0.000000000D+00 2.405433393D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.279011100D+05-1.212064449D+02

Ni(cr) Crystal Ref-Elm. <lambda trans 631K. Chase,1998 pp1697-700.  
 2 j12/76 NI 1.00 0.00 0.00 0.00 0.00 1 58.6934000 0.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4786.000  
 -7.689131090D+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 pp1697-700.  
 2 j12/76 NI 1.00 0.00 0.00 0.00 0.00 2 58.6934000 0.000  
 631.000 1200.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4786.000  
 1.036354737D+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 pp1697-700.  
 1 j12/76 NI 1.00 0.00 0.00 0.00 0.00 3 58.6934000 0.000  
 1728.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 4786.000  
 0.000000000D+00 0.000000000D+00 4.679890938D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.216258550D+02-2.335474714D+01

NiS(b) Beta. Chase,1998 pp1704-6.  
 1 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 1 90.7584000 -87864.000  
 200.000 652.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8465.000  
 9.281477840D+04-2.341897035D+03 2.156233266D+01-5.304222560D-02 9.993984760D-05  
 -9.111093130D-08 3.288570290D-11 -1.702746009D+03-1.117002463D+02

NiS(a) Alpha. Chase,1998 pp1704-6.  
 1 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 2 90.7584000 -87864.000  
 652.000 1249.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8465.000  
 2.424566967D+05-1.320914239D+03 7.077218200D+00 9.029383650D-05 2.068184040D-06  
 -6.559770780D-10 8.194048850D-14 -3.434758890D+03-3.562024750D+01

NiS(L) Liquid. Chase,1998 pp1704-6.  
 1 j12/76 NI 1.00S 1.00 0.00 0.00 0.00 3 90.7584000 -87864.000  
 1249.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8465.000  
 0.000000000D+00 0.000000000D+00 9.233977709D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.105334670D+04-4.576765033D+01

NiS<sub>2</sub>(cr) Crystal. Chase,1998 pp1708-10.  
 1 j 3/77 NI 1.00S 2.00 0.00 0.00 0.00 1 122.8234000 -131377.600  
 298.150 1280.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -1.676910840D+03 1.842877438D+01 7.671341480D+00 2.663682250D-03-1.892467189D-07  
 1.078337009D-10-2.438956464D-14 -1.831575942D+04-3.578715100D+01

NiS<sub>2</sub>(L) Liquid. Chase,1998 pp1708-10.  
 1 j 3/77 NI 1.00S 2.00 0.00 0.00 0.00 2 122.8234000 -131377.600  
 1280.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 0.000000000D+00 0.000000000D+00 1.094496248D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.234477669D+04-4.971946503D+01

## Appendix D (continued)

Ni3S2(a) Alpha. Pankratz,1987 p225-6. Chase,1998 pp1711-3 12/83.  
 1 g12/00 NI 3.00S 2.00 0.00 0.00 0.00 1 240.2102000 -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. Pankratz,1987 p225-6.  
 1 g12/00 NI 3.00S 2.00 0.00 0.00 0.00 2 240.2102000 -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. Pankratz,1987 p225-6.  
 1 g12/00 NI 3.00S 2.00 0.00 0.00 0.00 3 240.2102000 -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

Ni3S4(cr) Crystal. Chase,1998 p1714.  
 1 j 3/77 NI 3.00S 4.00 0.00 0.00 0.00 1 304.3402000 -301115.000  
 298.150 1100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 7.214883180D+03-7.806476430D+01 1.500658024D+01 1.653827825D-02 8.768311110D-07  
 -5.301784170D-10 1.279272852D-13 -4.096266670D+04-6.825975310D+01

P(cr) White. Ref-Elm. Gurvich,1989 pt1 p395 pt2 p326. Chase,1998a.  
 1 tpis89 P 1.00 0.00 0.00 0.00 0.00 1 30.9737610 0.000  
 195.400 317.3007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5360.000  
 -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 30.9737610 0.000  
 317.300 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5360.000  
 0.000000000D+00 0.000000000D+00 3.141496011D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.621436240D+02-1.272272999D+01

P4O10(cr) Crystal. Gurvich,1989 pt1 p417 pt2 p270.  
 2 tpis89 P 4.000 10.00 0.00 0.00 0.00 1 283.8890440 -3010100.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 34220.000  
 -2.910475984D+04 0.000000000D+00 5.209612140D+00 7.058407940D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.668178470D+05-2.310786251D+01  
 298.150 699.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 34220.000  
 0.000000000D+00 0.000000000D+00 5.461897334D+00 8.078166964D-02-4.072398734D-05  
 0.000000000D+00 0.000000000D+00 -3.668889200D+05-2.561194012D+01

P4O10(L) Liquid. Gurvich,1989 pt1 p417 pt2 p270.  
 1 tpis89 P 4.000 10.00 0.00 0.00 0.00 3 283.8890440 -3010100.000  
 699.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 34220.000  
 0.000000000D+00 0.000000000D+00 4.450051777D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.765523910D+05-2.311704609D+02

Pb(cr) Cubic. Ref-Elm. Gurvich,1991 pt1 p400 pt2 p337.  
 1 tpis91 PB 1.00 0.00 0.00 0.00 0.00 1 207.2000000 0.000  
 200.000 600.6507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6870.000  
 -6.149670140D+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 2 207.2000000 0.000  
 600.650 3600.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6870.000  
 -3.798179327D+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

PbBr2(cr) Rhombic Crystal. Gurvich,1991 pt1 p435 pt2 p361.  
 2 tpis91 PB 1.00BR 2.00 0.00 0.00 0.00 1 367.0080000 -276700.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19230.000  
 0.000000000D+00 0.000000000D+00 6.565717260D+00 1.959605208D-02-3.191530530D-05  
 0.000000000D+00 0.000000000D+00 -3.582576310D+04-2.245707569D+01  
 298.150 644.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19230.000  
 8.046174699D+00 0.000000000D+00 6.899264058D+00 5.925905435D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.532970360D+04-2.124769272D+01

PbBr2(L) Liquid. Gurvich,1991 pt1 p435 pt2 p361.  
 1 tpis91 PB 1.00BR 2.00 0.00 0.00 0.00 2 367.0080000 -276700.000  
 644.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19230.000  
 0.000000000D+00 0.000000000D+00 1.347042700D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.648036370D+04-5.695842618D+01

PbCL2(cr) Rhombic Crystal. Gurvich,1991 pt1 p428 pt2 p356.  
 1 tpis91 PB 1.00CL 2.00 0.00 0.00 0.00 1 278.1060000 -359400.000  
 200.000 774.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17150.000  
 2.697281121D+06-4.212942350D+04 2.651641932D+02-7.891350070D-01 1.316948609D-03  
 -1.123561948D-06 3.854416550D-10 1.522766773D+05-1.434661776D+03

## Appendix D (continued)

PbCL2(L) Liquid. Gurvich,1991 pt1 p428 pt2 p356.  
 1 tps91 PB 1.00CL 2.00 0.00 0.00 0.00 2 278.1060000 -359400.000  
 774.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17150.000  
 0.000000000D+00 0.000000000D+00 1.335015533D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.613690180D+04-5.953419614D+01

PbF2(II) Rhombic Crystal(II). Gurvich,1991 pt1 p421 pt2 p351.  
 1 tps91 PB 1.00F 2.00 0.00 0.00 0.00 1 245.1968064 -676000.000  
 298.150 583.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15000.000  
 1.363880734D+04 0.000000000D+00 7.104086711D+00 4.806777549D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.358963280D+04-2.908385048D+01

PbF2(I) Cubic Crystal(I). Gurvich,1991 pt1 p421 pt2 p351.  
 2 tps91 PB 1.00F 2.00 0.00 0.00 0.00 2 245.1968064 -676000.000  
 583.000 716.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15000.000  
 -7.862766417D+07 0.000000000D+00 1.154013526D+03-2.413080386D+00 1.453441514D-03  
 0.000000000D+00 0.000000000D+00 -5.720487300D+05-6.285579567D+03  
 716.000 1103.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15000.000  
 3.516663038D+07 0.000000000D+00-1.580925394D+02 1.905776769D-01-5.650555475D-05  
 0.000000000D+00 0.000000000D+00 4.370723820D+04 9.735936305D+02

PbF2(L) Liquid. Gurvich,1991 pt1 p421 pt2 p351.  
 1 tps91 PB 1.00F 2.00 0.00 0.00 0.00 3 245.1968064 -676000.000  
 1103.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15000.000  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.458950020D+04-6.282775717D+01

PbI2(cr) Hexagonal Crystal. Gurvich,1991 pt1 p441 pt2 p366.  
 2 tps91 PB 1.00I 2.00 0.00 0.00 0.00 1 461.0089400 -176000.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19500.000  
 -6.615857400D+03 0.000000000D+00 8.879658690D+00 1.758307313D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.391562477D+04-3.012466437D+01  
 298.150 683.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19500.000  
 4.428402876D+04 0.000000000D+00 7.731062925D+00 3.690055096D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.348831172D+04-2.387008226D+01

PbI2(L) Liquid. Gurvich,1991 pt1 p441 pt2 p366.  
 1 tps91 PB 1.00I 2.00 0.00 0.00 0.00 2 461.0089400 -176000.000  
 683.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19500.000  
 0.000000000D+00 0.000000000D+00 1.310961199D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.355165613D+04-5.237973135D+01

PbO(II-r) Tetragonal (II-red).Gurvich,1991 pt1 p409 pt2 p343.  
 2 tps91 PB 1.00O 1.00 0.00 0.00 0.00 1 223.1994000 -218600.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9225.000  
 0.000000000D+00 0.000000000D+00 8.050624580D-01 2.884978163D-02-4.302158100D-05  
 0.000000000D+00 0.000000000D+00 -2.743361905D+04-3.117085753D+00  
 298.150 762.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9225.000  
 -6.651023332D+03 0.000000000D+00 4.939557472D+00 2.406636110D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.789339075D+04-2.073932502D+01

PbO(I-y) Rhombic (I-yellow).Gurvich,1991 pt1 p409 pt2 p343.  
 1 tps91 PB 1.00O 1.00 0.00 0.00 0.00 2 223.1994000 -218600.000  
 762.000 1160.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9225.000  
 -3.360390450D+04 0.000000000D+00 5.407414267D+00 1.595644241D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.802576574D+04-2.321766400D+01

PbO(L) Liquid.Gurvich,1991 pt1 p409 pt2 p343.  
 1 tps91 PB 1.00O 1.00 0.00 0.00 0.00 3 223.1994000 -218600.000  
 1160.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9225.000  
 0.000000000D+00 0.000000000D+00 7.817658527D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.664258145D+04-3.570913839D+01

PbO2(cr) Tetragonal. Gurvich,1991 pt1 p415 p52 p346.  
 2 tps91 PB 1.00O 2.00 0.00 0.00 0.00 1 239.1988000 -276000.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10962.000  
 0.000000000D+00 0.000000000D+00 1.007530476D-01 4.035527600D-02-5.395750800D-05  
 0.000000000D+00 0.000000000D+00 -3.454199070D+04-1.557803514D+00  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10962.000  
 -2.593057198D+05 0.000000000D+00 1.010402297D+01 5.003301457D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.709944890D+04-5.052640331D+01

PbS(cr) Cubic. Gurvich,1991 pt1 p445 p52 p370.  
 2 tps91 PB 1.00S 1.00 0.00 0.00 0.00 1 239.2650000 -99474.800  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11510.000  
 -1.110196130D+04 0.000000000D+00 5.788552660D+00 9.715425300D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.377027529D+04-2.236417313D+01  
 298.150 1386.5007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11510.000  
 -7.529006520D+04 0.000000000D+00 7.331760982D+00-2.262310106D-03 1.609234940D-06  
 0.000000000D+00 0.000000000D+00 -1.431615352D+04-3.062514348D+01



## Appendix D (continued)

PbS(L) Liquid. Gurvich,1991 pt1 p445 p52 p370.  
 1 tpis91 PB 1.00S 1.00 0.00 0.00 0.00 2 239.2650000 -99474.800  
 1386.500 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11510.000  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.007241100D+04 -3.316574241D+01

Pb2O3(cr) Monoclinic. Gurvich,1991 pt1 p417 pt2 p348.  
 2 tpis91 PB 2.000 3.00 0.00 0.00 0.00 1 462.3982000 -491700.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20880.000  
 0.000000000D+00 0.000000000D+00 1.574967406D+00 6.633690300D-02 -9.449445980D-05  
 0.000000000D+00 0.000000000D+00 -6.172080000D+04 -6.282642160D+00  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20880.000  
 -3.314687215D+05 0.000000000D+00 1.505921576D+01 5.443495768D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.498118220D+04 -7.101946635D+01

Pb3O4(cr) Tetragonal. Gurvich,1991 pt1 p418 pt2 p349.  
 1 tpis91 PB 3.000 4.00 0.00 0.00 0.00 1 685.5976000 -720000.000  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 29830.000  
 7.031601470D+06 -8.770415980D+04 4.195886490D+02 -9.058738460D-01 1.138287119D-03  
 -7.358926050D-07 1.922732625D-10 3.431611340D+05 -2.394229365D+03

Rb(cr) Cubic. Ref-Elm. Cox,1989 p260. Chase,1998a p1849 12/83.  
 1 coda89 RB 1.00 0.00 0.00 0.00 0.00 1 85.4678000 0.000  
 100.000 312.4707 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7489.000  
 -1.693678854D+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 p260.  
 2 coda89 RB 1.00 0.00 0.00 0.00 0.00 2 85.4678000 0.000  
 312.470 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 7489.000  
 2.365752770D+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

RbBO2(b) Gurvich,1982 pt1 p458 pt2 p482.  
 2 tpis82 RB 1.00B 1.000 2.00 0.00 0.00 1 128.2776000 -975000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13310.000  
 1.320700184D+06 -2.114255330D+04 1.338015047D+02 -3.804509820D-01 6.570568430D-04  
 -5.884791840D-07 2.152384344D-10 -2.010026759D+04 -7.254857290D+02  
 500.000 968.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13310.000  
 -1.553422560D+05 0.000000000D+00 9.425074910D+00 3.853433670D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.207672511D+05 -4.437890740D+01

RbBO2(a) Gurvich,1982 pt1 p458 pt2 p482.  
 1 tpis82 RB 1.00B 1.000 2.00 0.00 0.00 2 128.2776000 -975000.000  
 968.000 1133.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13310.000  
 0.000000000D+00 0.000000000D+00 1.298934032D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.222516025D+05 -6.507104425D+01

RbBO2(L) Gurvich,1982 pt1 p458 pt2 p482.  
 1 tpis82 RB 1.00B 1.000 2.00 0.00 0.00 3 128.2776000 -975000.000  
 1133.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13310.000  
 0.000000000D+00 0.000000000D+00 1.743939210D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.235650894D+05 -9.307583456D+01

RbBr(cr) Cubic. Gurvich,1982 pt1 p445 pt2 p469.  
 1 tpis82 RB 1.00BR 1.00 0.00 0.00 0.00 1 165.3718000 -394770.000  
 200.000 965.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13060.000  
 -5.724525880D+04 9.082670760D+02 4.275929780D-01 1.751269798D-02 -2.421969308D-05  
 1.854230436D-08 -5.603980870D-12 -5.357247720D+04 9.232346100D+00

RbBr(L) Liquid. Gurvich,1982 pt1 p445 pt2 p469.  
 1 tpis82 RB 1.00BR 1.00 0.00 0.00 0.00 2 165.3718000 -394770.000  
 965.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13060.000  
 0.000000000D+00 0.000000000D+00 8.755777550D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.852456540D+04 -3.604442573D+01

RbCL(cr) Cubic. Gurvich,1982 pt1 p441 pt2 p466.  
 1 tpis82 RB 1.00CL 1.00 0.00 0.00 0.00 1 120.9208000 -435220.000  
 200.000 997.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12160.000  
 -5.731907690D+04 4.298433250D+02 4.955874940D+00 9.930643910D-04 3.857679940D-06  
 -4.516778380D-09 1.683809372D-12 -5.653364290D+04 -1.609477359D+01

RbCL(L) Liquid. Gurvich,1982 pt1 p441 pt2 p466.  
 1 tpis82 RB 1.00CL 1.00 0.00 0.00 0.00 2 120.9208000 -435220.000  
 997.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12160.000  
 0.000000000D+00 0.000000000D+00 8.827940552D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.345006300D+04 -3.845805693D+01

## Appendix D (continued)

RbF(cr) Cubic. Gurvich,1982 pt1 p438 pt2 p463.  
 1 tpis82 RB 1.00F 1.00 0.00 0.00 0.00 1 104.4662032 -559700.000  
 298.150 1068.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10900.000  
 5.640741306D+03 0.000000000D+00 5.092663308D+00 3.129949931D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.895462790D+04-2.057230003D+01

RbF(L) Liquid. Gurvich,1982 pt1 p438 pt2 p463.  
 1 tpis82 RB 1.00F 1.00 0.00 0.00 0.00 2 104.4662032 -559700.000  
 1068.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10900.000  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.775044270D+04-3.835948403D+01

RbH(cr) Cubic. Gurvich,1982 pt1 p434 pt2 p458.  
 1 tpis82 RB 1.00H 1.00 0.00 0.00 0.00 1 86.4757400 -52300.000  
 298.150 858.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9100.000  
 -6.384020225D+04 0.000000000D+00 4.263149602D+00 3.963552873D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.951554350D+03-1.816921793D+01

RbH(L) Liquid. Gurvich,1982 pt1 p434 pt2 p458.  
 1 tpis82 RB 1.00H 1.00 0.00 0.00 0.00 2 86.4757400 -52300.000  
 858.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9100.000  
 0.000000000D+00 0.000000000D+00 6.735213500D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.893290150D+03-2.833905350D+01

RbI(cr) Cubic. Gurvich,1982 pt1 p448 pt2 p472.  
 1 tpis82 RB 1.00I 1.00 0.00 0.00 0.00 1 212.3722700 -333600.000  
 200.000 929.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13340.000  
 -1.871461077D+05 2.207646572D+03-3.199388250D+00 1.739850250D-02-1.184152545D-05  
 3.313152520D-09 3.472456000D-13 -5.305010310D+04 3.417793530D+01

RbI(L) Liquid. Gurvich,1982 pt1 p448 pt2 p472.  
 1 tpis82 RB 1.00I 1.00 0.00 0.00 0.00 2 212.3722700 -333600.000  
 929.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13340.000  
 0.000000000D+00 0.000000000D+00 8.671587382D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.112940250D+04-3.435941214D+01

RbNO2(I) Cubic. Gurvich,1982 pt1 p453 pt2 p477.  
 1 tpis82 RB 1.00N 1.000 2.00 0.00 0.00 1 131.4733000 -367000.000  
 298.150 695.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23400.000  
 0.000000000D+00 0.000000000D+00 9.108895172D+00 3.333690139D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.700369140D+04-3.340874045D+01

RbNO2(L) Liquid. Gurvich,1982 pt1 p453 pt2 p477.  
 1 tpis82 RB 1.00N 1.000 2.00 0.00 0.00 2 131.4733000 -367000.000  
 695.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 23400.000  
 0.000000000D+00 0.000000000D+00 1.250825364D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.710583050D+04-5.124298955D+01

RbNO3(IV) Hexagonal. Gurvich,1982 pt1 p455 pt2 p479.  
 1 tpis82 RB 1.00N 1.000 3.00 0.00 0.00 1 147.4727000 -494700.000  
 200.000 437.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19640.000  
 1.211253372D+07-2.028159094D+05 1.325899840D+03-4.151421820D+00 6.401606600D-03  
 -3.822822630D-06 0.000000000D+00 8.768873850D+05-7.162144700D+03

RbNO3(III) Cubic. Gurvich,1982 pt1 p455 pt2 p479.  
 1 tpis82 RB 1.00N 1.000 3.00 0.00 0.00 2 147.4727000 -494700.000  
 437.000 493.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19640.000  
 0.000000000D+00 0.000000000D+00 9.120561524D+00 1.643716828D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.277664760D+04-3.918776498D+01

RbNO3(II) Hexagonal. Gurvich,1982 pt1 p455 pt2 p479.  
 1 tpis82 RB 1.00N 1.000 3.00 0.00 0.00 3 147.4727000 -494700.000  
 493.000 556.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19640.000  
 0.000000000D+00 0.000000000D+00 1.078616780D+02-2.821762196D-01 0.000000000D+00  
 3.922207081D-07 0.000000000D+00 -8.057470150D+04-5.191016028D+02

RbNO3(I) Cubic. Gurvich,1982 pt1 p455 pt2 p479.  
 1 tpis82 RB 1.00N 1.000 3.00 0.00 0.00 4 147.4727000 -494700.000  
 556.000 583.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19640.000  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.449488250D+04-8.253206472D+01

RbNO3(L) Liquid. Gurvich,1982 pt1 p455 pt2 p479.  
 1 tpis82 RB 1.00N 1.000 3.00 0.00 0.00 5 147.4727000 -494700.000  
 583.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19640.000  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.394163280D+04-8.158309442D+01

RbOH(b) Beta. Gurvich,1997.  
 1 g 8/97 RB 1.00O 1.00H 1.00 0.00 0.00 1 102.4751400 -418800.000  
 298.150 508.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13500.000  
 0.000000000D+00 0.000000000D+00 6.589925323D+00 5.731305874D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.258929920D+04-2.794998878D+01

## Appendix D (continued)

RbOH(c)                      Gamma. Gurvich,1997.  
 1 g 8/97 RB 1.000 1.00H 1.00 0.00 0.00 2 102.4751400 -418800.000  
 508.000 658.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13500.000  
 0.000000000D+00 0.000000000D+00 9.140646893D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.248404970D+04 -3.962855491D+01

RbOH(L)                      Liquid. Gurvich,1997.  
 1 g 8/97 RB 1.000 1.00H 1.00 0.00 0.00 3 102.4751400 -418800.000  
 658.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13500.000  
 0.000000000D+00 0.000000000D+00 1.034336359D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.231326390D+04 -4.597096049D+01

RbO2(b)                      Beta,hexagonal. Gurvich,1982 pt1 p430 pt2 p453.  
 1 tps82 RB 1.000 2.00 0.00 0.00 0.00 1 117.4666000 -279100.000  
 200.000 423.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16760.000  
 -5.914373690D+05 9.356154690D+03 -5.173703230D+01 1.872603527D-01 -2.664203296D-04  
 1.581120816D-07 0.000000000D+00 -7.971547560D+04 2.930911089D+02

RbO2(a)                      Alpha,cubic. Gurvich,1982 pt1 p430 pt2 p453.  
 1 tps82 RB 1.000 2.00 0.00 0.00 0.00 2 117.4666000 -279100.000  
 423.000 813.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16760.000  
 0.000000000D+00 0.000000000D+00 1.058390693D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.680173520D+04 -4.488768335D+01

RbO2(L)                      Liquid. Gurvich,1982 pt1 p430 pt2 p453.  
 1 tps82 RB 1.000 2.00 0.00 0.00 0.00 3 117.4666000 -279100.000  
 813.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16760.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.544940050D+04 -5.145193248D+01

Rb2CO3(a)                      Alpha,monoclinic. Gurvich,1982 pt1 p457 pt2 p481.  
 1 tps82 RB 2.00C 1.000 3.00 0.00 0.00 1 230.9445000 -1132600.000  
 200.000 576.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24480.000  
 -1.377487286D+06 2.415872404D+04 -1.620555595D+02 6.425655960D-01 -1.249826185D-03  
 1.304525231D-06 -5.552423710D-10 -2.500033904D+05 8.719586300D+02

Rb2CO3(b)                      Beta,hexagonal. Gurvich,1982 pt1 p457 pt2 p481.  
 1 tps82 RB 2.00C 1.000 3.00 0.00 0.00 2 230.9445000 -1132600.000  
 576.000 1146.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24480.000  
 0.000000000D+00 0.000000000D+00 1.355678206D+01 8.280944999D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.405896222D+05 -5.801044809D+01

Rb2CO3(L)                      Liquid. Gurvich,1982 pt1 457 pt2 p481.  
 1 tps82 RB 2.00C 1.000 3.00 0.00 0.00 3 230.9445000 -1132600.000  
 1146.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 24480.000  
 0.000000000D+00 0.000000000D+00 2.465569228D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.442630744D+05 -1.235531008D+02

Rb2O(c)                      Gamma,cubic. Gurvich,1982 pt1 p431 pt2 p454.  
 1 tps82 RB 2.000 1.00 0.00 0.00 0.00 1 186.9350000 -338000.000  
 298.150 543.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15600.000  
 0.000000000D+00 0.000000000D+00 6.190743652D+00 9.087246272D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.290149280D+04 -2.294776447D+01

Rb2O(b)                      Beta,cubic. Gurvich,1982 pt1 p431 pt2 p454.  
 1 tps82 RB 2.000 1.00 0.00 0.00 0.00 2 186.9350000 -338000.000  
 543.000 613.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15600.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.464679770D+04 -5.461093903D+01

Rb2O(a)                      Alpha,hexagonal. Gurvich,1982 pt1 p431 pt2 p454.  
 1 tps82 RB 2.000 1.00 0.00 0.00 0.00 3 186.9350000 -338000.000  
 613.000 778.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15600.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.416571100D+04 -5.382613205D+01

Rb2O(L)                      Liquid. Gurvich,1982 pt1 p431 pt2 p454.  
 1 tps82 RB 2.000 1.00 0.00 0.00 0.00 4 186.9350000 -338000.000  
 778.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15600.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.176027770D+04 -5.073431535D+01

Rb2O2(b)                      Beta,rhombic Gurvich,1982 pt1 p433 pt2 p456.  
 1 tps82 RB 2.000 2.00 0.00 0.00 0.00 1 202.9344000 -410000.000  
 298.150 398.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19700.000  
 0.000000000D+00 0.000000000D+00 2.566116344D+00 2.890861879D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.136136520D+04 -3.996333599D+00

Rb2O2(a)                      Alpha,cubic. Gurvich,1982 pt1 p433 pt2 p456.  
 1 tps82 RB 2.000 2.00 0.00 0.00 0.00 2 202.9344000 -410000.000  
 398.000 843.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19700.000  
 0.000000000D+00 0.000000000D+00 1.407178535D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.365100100D+04 -6.136883861D+01

## Appendix D (continued)

Rb2O2 (L) Liquid. Gurvich, 1982 pt1 p433 pt2 p456.

1	tpis82 RB	2.000	2.00	0.00	0.00	0.00	3	202.9344000	-410000.000
	843.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	1.611640373D+01	0.000000000D+00	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-5.284890920D+04-7.214727369D+01

Rb2SO4 (a) Alpha, rhombic. Gurvich, 1982 pt1 p451 pt2 p475.

3	tpis82 RB	2.00S	1.000	4.00	0.00	0.00	1	266.9982000	-1435900.000
	200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-1.192448350D+07	2.294293959D+05	-1.785117228D+03	7.309062720D+00	-1.617521748D-02				
	1.861676545D-05	-8.714648070D-09							-1.202291196D+06 9.289553650D+03
	500.000	800.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-4.871322610D+05	0.000000000D+00	2.853725036D+01	-3.587804810D-02	4.220439770D-05				
	0.000000000D+00	0.000000000D+00							-1.816178572D+05-1.327574146D+02
	800.000	931.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	3.464686434D+02	-6.082068577D-01	0.000000000D+00				
	3.246132364D-07	0.000000000D+00							-2.782463487D+05-1.841656965D+03

Rb2SO4 (b) Beta, hexagonal. Gurvich, 1982 pt1 p451 pt2 p475.

1	tpis82 RB	2.00S	1.000	4.00	0.00	0.00	2	266.9982000	-1435900.000
	931.000	1343.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	1.107353290D+01	1.230667833D-02	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-1.739435450D+05-3.919109508D+01

Rb2SO4 (L) Liquid. Gurvich, 1982 pt1 p451 pt2 p475.

1	tpis82 RB	2.00S	1.000	4.00	0.00	0.00	3	266.9982000	-1435900.000
	1343.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	2.483609978D+01	0.000000000D+00	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-1.768420750D+05-1.184499504D+02

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	32.0650000	0.000
	200.000	368.3007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-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	32.0650000	0.000
	368.300	388.3607	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	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	32.0650000	0.000
	388.360	428.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-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
	0.000000000D+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
	0.000000000D+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
	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
	0.000000000D+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

SCL2 (L) Chase, 1998 p855.

1	j 6/78 S	1.00CL	2.00	0.00	0.00	0.00	1	102.9710000	-49790.000
	298.150	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	1.094496248D+01	0.000000000D+00	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-9.251567000D+03-4.026872255D+01

S2CL2 (L) Chase, 1998 p858.

1	j 6/78 S	2.00CL	2.00	0.00	0.00	0.00	1	135.0360000	-58158.000
	298.150	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	1.494856582D+01	0.000000000D+00	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-1.145167466D+04-5.824880790D+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	44.9559100	0.000
	100.000	400.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-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
	-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

## Appendix D (continued)

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	44.9559100	0.000
	1609.000	1814.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	5.316007798D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+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	44.9559100	0.000
	1814.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	5.291953464D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00							-1.373974847D+03-2.764152183D+01

Sc2O3(cr)               Cubic. Gurvich,1982 pt1 p145 pt2 p150.

2	tpis82 SC	2.000	3.00	0.00	0.00	0.00	1	137.9100200	-1908600.000
	200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-2.372563268D+06	4.573798990D+04	-3.655376590D+02	1.588230977D+00	-3.584389210D-03				
	4.185870320D-06	-1.985472581D-09							-4.353786390D+05 1.884709407D+03
	500.000	2762.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-2.669869135D+05	0.000000000D+00	1.386002327D+01	1.535415402D-03	1.928963573D-07				
	0.000000000D+00	0.000000000D+00							-2.346482672D+05-7.170005710D+01

Sc2O3(L)               Liquid. Gurvich,1982 pt1 p145 pt2 p150.

1	tpis82 SC	2.000	3.00	0.00	0.00	0.00	2	137.9100200	-1908600.000
	2762.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	2.405433393D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00							-2.402224225D+05-1.419525042D+02

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	28.0855000	0.000
	200.000	298.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-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
	-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

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	28.0855000	0.000
	1690.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	3.271389414D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00							4.882667110D+03-1.326611073D+01

SiC(b)                   Beta,cubic. Gurvich,1991 pt1 p298 pt2 p264.

2	tpis91 SI	1.00C	1.00	0.00	0.00	0.00	1	40.0962000	-73000.000
	100.000	298.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-2.285496383D+03	0.000000000D+00	-5.349100620D-01	1.271547084D-02	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-9.193174900D+03 1.241441354D+00
	298.150	3105.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-1.269106658D+05	0.000000000D+00	3.757286960D+00	3.481744565D-03	-1.620660748D-06				
	2.611097948D-10	0.000000000D+00							-1.046667760D+04-2.109198538D+01

SiC(L)                   Liquid. Gurvich,1991 pt1 p298 pt2 p264.

1	tpis91 SI	1.00C	1.00	0.00	0.00	0.00	2	40.0962000	-73000.000
	3103.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	7.577115188D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00							-7.787459000D+03-4.367596159D+01

SiO2(a-qz)              Alpha-quartz,hexagonal. Gurvich,1991 pt1 p250 pt2 p228.

1	tpis91 SI	1.000	2.00	0.00	0.00	0.00	1	60.0843000	-910700.000
	200.000	848.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-5.776895500D+05	7.214661110D+03	-3.145730294D+01	7.412177150D-02	-8.670077820D-06				
	-1.080461312D-07	8.316324910D-11							-1.462398375D+05 1.842424399D+02

SiO2(b-qz)              Beta-quartz,hexagonal. Gurvich,1991 pt1 p250 pt2 p228.

1	tpis91 SI	1.000	2.00	0.00	0.00	0.00	2	60.0843000	-910700.000
	848.000	1200.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	2.317635074D+04	0.000000000D+00	7.026511484D+00	1.241925261D-03	0.000000000D+00				
	0.000000000D+00	0.000000000D+00							-1.117012474D+05-3.580751356D+01

SiO2(b-crt)              Beta-cristobalite,cubic. Gurvich,1991 pt1 p250 pt2 p228.

1	tpis91 SI	1.000	2.00	0.00	0.00	0.00	3	60.0843000	-910700.000
	1200.000	1996.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	-5.356419079D+05	0.000000000D+00	9.331036946D+00	-7.306503931D-04	3.339944266D-07				
	0.000000000D+00	0.000000000D+00							-1.134326721D+05-4.998768383D+01

SiO2(L)                   Liquid. Gurvich,1991 pt1 p250 pt2 p228.

1	tpis91 SI	1.000	2.00	0.00	0.00	0.00	4	60.0843000	-910700.000
	1996.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
	0.000000000D+00	0.000000000D+00	1.004268442D+01	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00	0.000000000D+00
	0.000000000D+00	0.000000000D+00							-1.140002976D+05-5.554279592D+01

## Appendix D (continued)

SiS(cr) Crystal. Gurvich,1991 pt1 p289 pt2 p257.  
 1 tpis91 SI 1.00S 1.00 0.00 0.00 0.00 1 60.1505000 -168737.210  
 298.150 1363.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9000.490  
 0.000000000D+00 0.000000000D+00 4.873408054D+00 1.807202108D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.182763678D+04-2.072841584D+01

SiS(L) Liquid. Gurvich,1991 pt1 p289 pt2 p257.  
 1 tpis91 SI 1.00S 1.00 0.00 0.00 0.00 2 60.1505000 -168737.210  
 1363.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 9000.490  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.076140696D+04-3.851581605D+01

SiS2(cr) Tetragonal. Gurvich,1991 pt1 p293 pt2 p259.  
 2 tpis91 SI 1.00S 2.00 0.00 0.00 0.00 1 92.2155000 -287000.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11180.490  
 -1.489679569D+04 0.000000000D+00 3.921710460D+00 1.226970632D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.628253940D+04-1.684224727D+01  
 298.150 1363.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11180.490  
 0.000000000D+00 0.000000000D+00 6.423349061D+00 3.317212921D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.658052990D+04-2.834259902D+01

SiS2(L) Liquid. Gurvich,1991 pt1 p293 pt2 p259.  
 1 tpis91 SI 1.00S 2.00 0.00 0.00 0.00 2 92.2155000 -287000.000  
 1363.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11180.490  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.909260770D+04-6.276638967D+01

Si2N2O(cr) Fegley,1981.  
 2 g 7/95 SI 2.00N 2.000 1.00 0.00 0.00 1 100.1838000 -947700.000  
 298.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -7.783293180D+06 7.787697680D+04-3.226727260D+02 7.513788890D-01-9.139450720D-04  
 5.774402010D-07-1.479973902D-10 -5.139865410D+05 1.873124449D+03  
 1000.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 0.000  
 -7.414096340D+06 2.559424417D+04-2.535540920D+01 3.208894230D-02-1.340182230D-05  
 3.075006784D-09-2.892800339D-13 -2.762647725D+05 1.907774092D+02

Si3N4(cr) Hexagonal. Gurvich,1991 pt1 p297 pt2 p262.  
 2 tpis91 SI 3.00N 4.00 0.00 0.00 0.00 1 140.2833000 -787800.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12113.490  
 -1.136434515D+04 0.000000000D+00-4.993435710D-01 3.962318940D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.640037870D+04-1.086768954D+00  
 298.150 4000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 12113.490  
 -2.910454134D+05 0.000000000D+00 1.189210188D+01 9.349799327D-03-2.551082385D-06  
 2.857654871D-10 0.000000000D+00 -9.966541740D+04-6.412447976D+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 1 118.7100000 0.000  
 200.000 505.1187 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6323.000  
 -9.970568110D+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 2 118.7100000 0.000  
 505.118 4700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6323.000  
 9.847844311D+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

SnBr2(cr) Rhombic. Gurvich,1991 pt1 p379 pt2 p322.  
 2 tpis91 SN 1.00BR 2.00 0.00 0.00 0.00 1 278.5180000 -253600.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18670.000  
 -1.072142073D+04 0.000000000D+00 8.650388720D+00 3.246938990D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.326028440D+04-3.191324070D+01  
 298.150 503.4007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18670.000  
 1.596365871D+05 0.000000000D+00 4.310656912D+00 1.137469316D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.175626170D+04-8.652273965D+00

SnBr2(L) Liquid. Gurvich,1991 pt1 p379 pt2 p322.  
 2 tpis91 SN 1.00BR 2.00 0.00 0.00 0.00 2 278.5180000 -253600.000  
 503.400 860.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18670.000  
 2.804494793D+05 0.000000000D+00 1.427732963D+01-2.218170403D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.305162210D+04-6.008238208D+01  
 860.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18670.000  
 0.000000000D+00 0.000000000D+00 1.274879698D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.288346740D+04-5.185141223D+01

SnBr4(cr) Monoclinic. Gurvich,1991 pt1 p382 pt2 p325.  
 1 tpis91 SN 1.00BR 4.00 0.00 0.00 0.00 1 438.3260000 -388000.000  
 200.000 302.2507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31260.000  
 -3.870038960D+06 0.000000000D+00 3.663330300D+02-1.775658617D+00 2.504656832D-03  
 0.000000000D+00 0.000000000D+00 -1.120730416D+05-1.659626236D+03

## Appendix D (continued)

SnBr<sub>4</sub>(L) Liquid. Gurvich,1991 pt1 p382 pt2 p325.  
 2 tps91 SN 1.00BR 4.00 0.00 0.00 0.00 2 438.3260000 -388000.000  
 302.250 470.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31260.000  
 1.124780655D+05 0.000000000D+00 1.859869072D+01-4.792826035D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.036569340D+04-6.913668591D+01  
 470.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31260.000  
 0.000000000D+00 0.000000000D+00 1.888265213D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.079140710D+04-7.136367786D+01

SnCL<sub>2</sub>(cr) Rhombic. Gurvich,1991 pt1 p372 pt2 p316.  
 1 tps91 SN 1.00CL 2.00 0.00 0.00 0.00 1 189.6160000 -333000.000  
 200.000 520.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17330.000  
 -3.455659100D+05 5.121048940D+03-2.179939832D+01 8.738265750D-02-1.087380837D-04  
 5.701191040D-08 0.000000000D+00 -6.692353080D+04 1.338412221D+02

SnCL<sub>2</sub>(L) Liquid. Gurvich,1991 pt1 p372 pt2 p316.  
 1 tps91 SN 1.00CL 2.00 0.00 0.00 0.00 2 189.6160000 -333000.000  
 520.200 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17330.000  
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.294240400D+04-5.766924967D+01

SnCL<sub>4</sub>(L) Liquid. Gurvich,1991 pt1 p375 pt2 p319.  
 2 tps91 SN 1.00CL 4.00 0.00 0.00 0.00 1 260.5220000 -517000.000  
 239.050 350.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38740.000  
 0.000000000D+00 0.000000000D+00 2.059050984D+01-5.567014773D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.807207820D+04-8.378462335D+01  
 350.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 38740.000  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.773111750D+04-7.431947542D+01

SnF<sub>2</sub>(cr) Monoclinic. Gurvich,1991 pt1 p367 pt2 p311.  
 1 tps91 SN 1.00F 2.00 0.00 0.00 0.00 1 156.7068064 -677000.000  
 298.150 488.2007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14200.000  
 0.000000000D+00 0.000000000D+00 6.575252180D+00 7.150150760D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.370213250D+04-2.802481800D+01

SnF<sub>2</sub>(L) Liquid. Gurvich,1991 pt1 p367 pt2 p311.  
 1 tps91 SN 1.00F 2.00 0.00 0.00 0.00 2 156.7068064 -677000.000  
 488.200 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14200.000  
 0.000000000D+00 0.000000000D+00 1.202716700D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.424882400D+04-5.569866810D+01

SnI<sub>2</sub>(cr) Monoclinic. Gurvich,1991 pt1 p386 pt2 p328.  
 1 tps91 SN 1.00I 2.00 0.00 0.00 0.00 1 372.5189400 -153000.000  
 200.000 595.7007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18950.000  
 8.194427570D+05-1.285027272D+04 8.314392190D+01-1.959449848D-01 2.384765022D-04  
 -9.891789320D-08 0.000000000D+00 3.957086730D+04-4.432502620D+02

SnI<sub>2</sub>(L) Liquid. Gurvich,1991 pt1 p386 pt2 p328.  
 2 tps91 SN 1.00I 2.00 0.00 0.00 0.00 2 372.5189400 -153000.000  
 595.700 960.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18950.000  
 3.807680789D+05 0.000000000D+00 1.313799611D+01-7.105650243D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.013964325D+04-5.193401798D+01  
 960.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18950.000  
 0.000000000D+00 0.000000000D+00 1.286906865D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.060553468D+04-5.097603343D+01

SnI<sub>4</sub>(cr) Cubic. Gurvich,1991 pt1 p389 pt2 p331  
 1 tps91 SN 1.00I 4.00 0.00 0.00 0.00 1 626.3278800 -207500.000  
 200.000 418.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31600.000  
 1.365815960D+06-2.186441599D+04 1.411768692D+02-3.151970333D-01 2.991203201D-04  
 0.000000000D+00 0.000000000D+00 7.347422460D+04-7.553382720D+02

SnI<sub>4</sub>(L) Liquid. Gurvich,1991 pt1 p389 pt2 p331  
 2 tps91 SN 1.00I 4.00 0.00 0.00 0.00 2 626.3278800 -207500.000  
 418.000 580.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31600.000  
 3.125499879D+05 0.000000000D+00 2.114568387D+01-5.918328320D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.828678876D+04-7.927900653D+01  
 580.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31600.000  
 0.000000000D+00 0.000000000D+00 1.864210880D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.836905732D+04-6.724586950D+01

SnO(cr) Tetragonal. Gurvich,1991 pt1 p356 pt2 p306.  
 2 tps91 SN 1.00O 1.00 0.00 0.00 0.00 1 134.7094000 -280710.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8736.000  
 0.000000000D+00 0.000000000D+00 7.279467580D-02 3.307685420D-02-4.710942000D-05  
 0.000000000D+00 0.000000000D+00 -3.483713220D+04-1.306828645D+00  
 298.150 1250.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8736.000  
 0.000000000D+00 0.000000000D+00 5.260682830D+00 1.630883840D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.540242040D+04-2.358356588D+01

## Appendix D (continued)

SnO(L) Liquid. Gurvich,1991 pt1 p356 pt2 p306.  
 1 tpis91 SN 1.000 1.00 0.00 0.00 0.00 2 134.7094000 -280710.000  
 1250.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8736.000  
 0.000000000D+00 0.000000000D+00 7.577115188D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.369230760D+04 -3.539798567D+01  
 SnO2(cr) Tetragonal. Gurvich,1991 pt1 p361 pt2 p308.  
 2 tpis91 SN 1.000 2.00 0.00 0.00 0.00 1 150.7088000 -577630.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8384.000  
 0.000000000D+00 0.000000000D+00 -1.177647966D+00 3.970167880D-02 -4.790758920D-05  
 0.000000000D+00 0.000000000D+00 -7.046277710D+04 2.896556966D+00  
 298.150 1903.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8384.000  
 -2.674601390D+05 0.000000000D+00 9.145457760D+00 8.856805753D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.313567410D+04 -4.798106778D+01  
 SnO2(L) Liquid. Gurvich,1991 pt1 p361 pt2 p308.  
 1 tpis91 SN 1.000 2.00 0.00 0.00 0.00 2 150.7088000 -577630.000  
 1903.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8384.000  
 0.000000000D+00 0.000000000D+00 1.106499361D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.222994130D+04 -5.927455845D+01  
 SnS(cr) Rhombic. Gurvich,1991 pt1 p392 pt2 p333.  
 2 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 1 150.7750000 -109662.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10530.000  
 -1.473490121D+04 0.000000000D+00 5.317316410D+00 2.586688381D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.493898062D+04 -2.188910671D+01  
 298.150 875.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10530.000  
 3.056103126D+04 0.000000000D+00 4.511751143D+00 3.579405160D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.459100103D+04 -1.734052255D+01  
 SnS(cr) Cubic. Gurvich,1991 pt1 p392 pt2 p333.  
 1 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 2 150.7750000 -109662.000  
 875.000 1154.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10530.000  
 0.000000000D+00 0.000000000D+00 4.921516722D+00 1.882251630D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.425419920D+04 -1.855922147D+01  
 SnS(L) Liquid. Gurvich,1991 pt1 p392 pt2 p333.  
 1 tpis91 SN 1.00S 1.00 0.00 0.00 0.00 3 150.7750000 -109662.000  
 1154.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10530.000  
 0.000000000D+00 0.000000000D+00 9.008348057D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.391650549D+04 -4.190990669D+01  
 SnS2(cr) Hexagonal. Gurvich,1991 pt1 p396 pt2 p335.  
 2 tpis91 SN 1.00S 2.00 0.00 0.00 0.00 1 182.8400000 -141837.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13310.000  
 -2.817980768D+04 0.000000000D+00 6.586339710D+00 7.259692260D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.943987500D+04 -2.933754416D+01  
 298.150 1143.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13310.000  
 1.193094963D+04 0.000000000D+00 7.560277154D+00 2.479641013D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.938326475D+04 -3.323586315D+01  
 Sr(a) Alpha. Ref-Elm. Alcock,1993.  
 2 srd 93 SR 1.00 0.00 0.00 0.00 0.00 1 87.6200000 0.000  
 100.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6558.289  
 -4.150245670D+03 1.559823384D+02 -2.623173257D-01 2.945369354D-02 -1.212940361D-04  
 2.401045642D-07 -1.708772572D-10 -1.455791066D+03 3.435106060D+00  
 298.150 820.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6558.289  
 1.294412876D+05 -1.646179180D+03 1.111114164D+01 -1.973737192D-02 2.910871519D-05  
 -2.163423606D-08 6.508160860D-12 7.160398040D+03 -5.671602200D+01  
 Sr(b) Beta. Ref-Elm. Alcock,1993.  
 1 srd 93 SR 1.00 0.00 0.00 0.00 0.00 2 87.6200000 0.000  
 820.000 1041.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6558.289  
 0.000000000D+00 0.000000000D+00 3.190326309D+00 4.837326553D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.560991280D+02 -1.157238431D+01  
 Sr(L) Liquid. Ref-Elm. Alcock,1993.  
 1 srd 93 SR 1.00 0.00 0.00 0.00 0.00 3 87.6200000 0.000  
 1041.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6558.289  
 0.000000000D+00 0.000000000D+00 4.450051777D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.431940390D+02 -1.889703393D+01  
 SrBr2(a) Alpha,tetragonal. Gurvich,1996a pt1 p523 pt2 p403.  
 1 tpis96 SR 1.00BR 2.00 0.00 0.00 0.00 1 247.4280000 -722000.000  
 200.000 918.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18060.499  
 -1.563862878D+05 2.048387286D+03 -2.389924996D+00 3.200996340D-02 -4.324517230D-05  
 3.247344210D-08 -9.786717550D-12 -9.941922340D+04 2.897007516D+01



## Appendix D (continued)

SrBr2(b)                   Beta, Gurvich,1996a pt1 p523 pt2 p403.  
 1 tps96 SR 1.00BR 2.00 0.00 0.00 0.00 2 247.4280000 -722000.000  
 918.000 930.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18060.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -9.021650510D+04-5.212663905D+01

SrBr2(L)                   Liquid, Gurvich,1996a pt1 p523 pt2 p403.  
 1 tps96 SR 1.00BR 2.00 0.00 0.00 0.00 3 247.4280000 -722000.000  
 930.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18060.499  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -8.900176120D+04-5.082046285D+01

SrCO3(a)                   Alpha,rhombic, Gurvich,1996a pt1 p532 pt2 p411.  
 2 tps96 SR 1.00C 1.000 3.00 0.00 0.00 1 147.6289000 -1226000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15120.499  
 -3.185109310D+07 5.983944250D+05-4.555778730D+03 1.807422903D+01-3.922550990D-02  
 4.443338240D-05-2.057838162D-08 -2.840270234D+06 2.379927032D+04  
 500.000 1198.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15120.499  
 -4.737741611D+05 0.000000000D+00 1.829247905D+01-1.342833192D-02 1.073412624D-05  
 0.000000000D+00 0.000000000D+00 -1.539939771D+05-9.167197246D+01

SrCO3(b)                   Beta,rhombic, Gurvich,1996a pt1 p532 pt2 p411.  
 1 tps96 SR 1.00C 1.000 3.00 0.00 0.00 2 147.6289000 -1226000.000  
 1198.000 1689.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15120.499  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.541962605D+05-9.302015968D+01

SrCO3(c)                   Gamma,cubic, Gurvich,1996a pt1 p532 pt2 p411.  
 1 tps96 SR 1.00C 1.000 3.00 0.00 0.00 3 147.6289000 -1226000.000  
 1689.000 1767.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15120.499  
 0.000000000D+00 0.000000000D+00 1.755966377D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.541962605D+05-9.302015968D+01

SrCO3(L)                   Liquid, Gurvich,1996a pt1 p532 pt2 p411.  
 1 tps96 SR 1.00C 1.000 3.00 0.00 0.00 4 147.6289000 -1226000.000  
 1767.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15120.499  
 0.000000000D+00 0.000000000D+00 1.984482549D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.534232745D+05-1.073837834D+02

SrCL2(a)                   Alpha,cubic, Gurvich,1996a pt1 p518 pt2 p400.  
 2 tps96 SR 1.00CL 2.00 0.00 0.00 0.00 1 158.5260000 -833000.000  
 200.000 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16230.000  
 -8.219302560D+05 1.414627236D+04-9.066868860D+01 3.537351300D-01-6.601840230D-04  
 6.294183590D-07-2.405335168D-10 -1.675299882D+05 4.920219760D+02  
 700.000 990.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16230.000  
 1.112527665D+09 0.000000000D+00-1.718772952D+04 4.254819093D+01-3.935556431D-02  
 1.290928281D-05 0.000000000D+00 6.824931370D+06 9.213791630D+04

SrCL2(b)                   Beta,cubic, Gurvich,1996a pt1 p518 pt2 p400.  
 1 tps96 SR 1.00CL 2.00 0.00 0.00 0.00 2 158.5260000 -833000.000  
 900.000 1147.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16230.000  
 2.652616089D+08 0.000000000D+00-6.137593196D+02 3.705888862D-01 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 6.013938810D+05 4.028366895D+03

SrCL2(L)                   Liquid, Gurvich,1996a pt1 p518 pt2 p400.  
 1 tps96 SR 1.00CL 2.00 0.00 0.00 0.00 3 158.5260000 -833000.000  
 1147.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 16230.000  
 -1.621863465D+06 0.000000000D+00 1.278463794D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.040518221D+05-6.010500872D+01

SrF2(a)                   Alpha,cubic, Gurvich,1996a pt1 p513 pt2 p396.  
 2 tps96 SR 1.00F 2.00 0.00 0.00 0.00 1 125.6168064 -1229000.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13075.000  
 -1.436181472D+04-3.902704550D+02 9.084528850D+00 4.747017010D-03-9.922331280D-06  
 1.169135473D-08-4.825603120D-12 -1.484911532D+05-4.433988680D+01  
 800.000 1484.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13075.000  
 -1.706744719D+07 2.576630531D+04 3.257893350D+01-3.032276697D-02-2.832102640D-05  
 2.982419101D-08-2.378577761D-12 -3.511043830D+05-1.514196992D+02

SrF2(b)                   Beta,cubic, Gurvich,1996a pt1 p513 pt2 p396.  
 1 tps96 SR 1.00F 2.00 0.00 0.00 0.00 2 125.6168064 -1229000.000  
 1484.000 1750.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13075.000  
 5.274154560D+09-9.287005960D+04-1.188369557D+04 9.829240680D+00-2.277347958D-03  
 0.000000000D+00 0.000000000D+00 1.339064905D+07 7.586298750D+04

SrF2(L)                   Liquid, Gurvich,1996a pt1 p515 pt2 p396.  
 1 tps96 SR 1.00F 2.00 0.00 0.00 0.00 3 125.6168064 -1229000.000  
 1750.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13075.000  
 0.000000000D+00 0.000000000D+00 1.190689530D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.478877648D+05-5.796718683D+01

## Appendix D (continued)

SrH2(a)                    Alpha, rhombic. Gurvich, 1996a pt1 p501 pt2 p389.  
 1 tps96 SR 1.00H 2.00 0.00 0.00 0.00 1 89.6358800 -180000.000  
 298.000 1128.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8000.499  
 0.000000000D+00 0.000000000D+00 4.125438541D+00 3.912437414D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.305279501D+04 -1.841745147D+01

SrH2(b)                    Beta. Gurvich, 1996a pt1 p501 pt2 p389.  
 1 tps96 SR 1.00H 2.00 0.00 0.00 0.00 2 89.6358800 -180000.000  
 1128.000 1323.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8000.499  
 0.000000000D+00 0.000000000D+00 8.539288545D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.467660041D+04 -4.425795748D+01

SrH2(L)                    Liquid. Gurvich, 1996a pt1 p501 pt2 p389.  
 1 tps96 SR 1.00H 2.00 0.00 0.00 0.00 3 89.6358800 -180000.000  
 1323.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8000.499  
 0.000000000D+00 0.000000000D+00 9.020375224D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.254682969D+04 -4.562495289D+01

SrI2(cr)                    Rhombic. Gurvich, 1996a pt1 p527 pt2 p406.  
 1 tps96 SR 1.00I 2.00 0.00 0.00 0.00 1 341.4289400 -568000.000  
 200.000 811.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18920.499  
 -8.531836590D+05 1.396294943D+04 -8.134381170D+01 2.923620048D-01 -4.941293260D-04  
 4.280629170D-07 -1.479234641D-10 -1.358835709D+05 4.559376890D+02

SrI2(L)                    Liquid. Gurvich, 1996a pt1 p527 pt2 p406.  
 1 tps96 SR 1.00I 2.00 0.00 0.00 0.00 2 341.4289400 -568000.000  
 811.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18920.499  
 0.000000000D+00 0.000000000D+00 1.322988366D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.143040870D+04 -5.646969655D+01

SrO(cr)                    Cubic. Gurvich, 1996a pt1 p494 pt2 p383.  
 3 tps96 SR 1.00O 1.00 0.00 0.00 0.00 1 103.6194000 -591000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.499  
 -1.625438799D+06 2.932375088D+04 -2.136643281D+02 8.526581540D-01 -1.819594223D-03  
 2.035599655D-06 -9.340883290D-10 -2.053069998D+05 1.123784285D+03  
 500.000 1800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.499  
 -3.410904551D+04 0.000000000D+00 5.049245235D+00 3.431471007D-03 -3.042151612D-06  
 9.069686608D-10 0.000000000D+00 -7.282782040D+04 -2.317163697D+01  
 1800.000 2805.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.499  
 -3.971117961D+07 0.000000000D+00 7.850733236D+01 -5.336790743D-02 1.125297823D-05  
 0.000000000D+00 0.000000000D+00 -1.604896850D+05 -4.990588969D+02

SrO(L)                    Liquid. Gurvich, 1996a pt1 p494 pt2 p383.  
 1 tps96 SR 1.00O 1.00 0.00 0.00 0.00 2 103.6194000 -591000.000  
 2805.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.499  
 0.000000000D+00 0.000000000D+00 1.010282025D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -7.188203330D+04 -5.541556063D+01

Sr(OH)2(b)                Beta, tetragonal. Gurvich, 1996a pt1 p505 pt2 p392.  
 1 tps96 SR 1.00O 2.00H 2.00 0.00 0.00 1 121.6346800 -964300.000  
 200.000 753.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15272.499  
 5.749774650D+05 -9.564782420D+03 6.310466570D+01 -1.470270543D-01 2.468488663D-04  
 -2.041763520D-07 6.865596260D-11 -7.364279180D+04 -3.424340180D+02

Sr(OH)2(a)                Alpha. Gurvich, 1996a pt1 p505 pt2 p392.  
 1 tps96 SR 1.00O 2.00H 2.00 0.00 0.00 2 121.6346800 -964300.000  
 753.000 808.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15272.499  
 0.000000000D+00 0.000000000D+00 1.563531705D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.216576455D+05 -8.006737394D+01

Sr(OH)2(L)                Liquid. Gurvich, 1996a pt1 p505 pt2 p392.  
 1 tps96 SR 1.00O 2.00H 2.00 0.00 0.00 3 121.6346800 -964300.000  
 808.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 15272.499  
 0.000000000D+00 0.000000000D+00 1.840156546D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.211265258D+05 -9.516262078D+01

SrS(cr)                    Cubic. Gurvich, 1996a pt1 p528 pt2 p408.  
 2 tps96 SR 1.00S 1.00 0.00 0.00 0.00 1 119.6850000 -480000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10040.499  
 2.688173776D+06 -5.010846740D+04 3.813026790D+02 -1.462623236D+00 3.138875273D-03  
 -3.522660370D-06 1.619531388D-09 1.665724752D+05 -1.992760719D+03  
 500.000 2500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10040.499  
 -1.221960164D+04 0.000000000D+00 5.716873273D+00 9.316243531D-04 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.951728090D+04 -2.471633956D+01

SrS(L)                    Liquid. Gurvich, 1996a pt1 p528 pt2 p408.  
 1 tps96 SR 1.00S 1.00 0.00 0.00 0.00 2 119.6850000 -480000.000  
 2500.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 10040.499  
 0.000000000D+00 0.000000000D+00 8.058201866D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -5.487727330D+04 -3.767411768D+01

## Appendix D (continued)

SrS04(a)                    Alpha,Rhombic. Gurvich,1996a pt1 p531 pt2 p410.  
 1 tps96 SR    1.00S    1.000    4.00    0.00    0.00 1    183.6826000    -1457000.000  
 298.150    1430.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18400.499  
 -2.524863161D+05 0.000000000D+00 1.319271972D+01 6.424070691D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -1.803016041D+05-6.394942426D+01

SrS04(b)                    Beta,hexagonal. Gurvich,1996a pt1 p531 pt2 p410.  
 1 tps96 SR    1.00S    1.000    4.00    0.00    0.00 2    183.6826000    -1457000.000  
 1430.000    1880.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18400.499  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -1.827264862D+05-1.065597408D+02

SrS04(L)                    Liquid. Gurvich,1996a pt1 p531 pt2 p410.  
 1 tps96 SR    1.00S    1.000    4.00    0.00    0.00 3    183.6826000    -1457000.000  
 1880.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    18400.499  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -1.783967061D+05-1.042566663D+02

Ta(cr)                    Crystal. Ref-Elm. Chase,1998 pp1899-1901.  
 3 j12/72 TA    1.00    0.00    0.00    0.00    0.00 1    180.9479000    0.000  
 200.000    1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    5681.000  
 1.519941999D+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 pp1899-1901.  
 1 j12/72 TA    1.00    0.00    0.00    0.00    0.00 2    180.9479000    0.000  
 3258.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    5681.000  
 0.000000000D+00 0.000000000D+00 5.032166658D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -7.436042760D+02-2.597362534D+01

TaC(cr)                    Chase,1998 pp652-4.  
 2 j12/73 TA    1.00C    1.00    0.00    0.00    0.00 1    192.9586000    -144096.960  
 200.000    800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    6514.488  
 -1.182153887D+04 2.152843262D+02-1.710781252D+00 3.226351270D-02-6.059170690D-05  
 5.540177420D-08-1.961814434D-11    -1.908587628D+04 8.122034510D+00  
 800.000    4273.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    6514.488  
 -1.540090534D+05 2.156690707D+02 5.001633620D+00 1.161840292D-03-1.062186764D-07  
 2.082367078D-11-1.580991193D-15    -2.062101769D+04-2.388952788D+01

TaC(L)                    Chase,1998 pp652-4.  
 1 j12/73 TA    1.00C    1.00    0.00    0.00    0.00 2    192.9586000    -144096.960  
 4273.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    6514.488  
 0.000000000D+00 0.000000000D+00 8.051466653D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -1.010399602D+04-4.208381497D+01

Ta2O5(II)                    Rhombic. Gurvich,1982 pt1 p91 pt2 p92.  
 2 tps82 TA    2.000    5.00    0.00    0.00    0.00 1    441.8928000    -2049000.000  
 200.000    500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22950.000  
 -3.279677980D+06 6.126833460D+04-4.710233330D+02 1.998455231D+00-4.425553760D-03  
 5.098341430D-06-2.392974558D-09    -5.247547580D+05 2.448363106D+03  
 500.000    1633.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22950.000  
 -2.735481912D+05 0.000000000D+00 1.819193368D+01 3.735655440D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -2.529440756D+05-8.923622860D+01

Ta2O5(I)                    Monoclinic. Gurvich,1982 pt1 p91 pt2 p92.  
 1 tps82 TA    2.000    5.00    0.00    0.00    0.00 2    441.8928000    -2049000.000  
 1633.000    2150.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22950.000  
 0.000000000D+00 0.000000000D+00 2.525705063D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -2.590924400D+05-1.352062771D+02

Ta2O5(L)                    Liquid. Gurvich,1982 pt1 p91 pt2 p92.  
 1 tps82 TA    2.000    5.00    0.00    0.00    0.00 3    441.8928000    -2049000.000  
 2150.000    6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    22950.000  
 0.000000000D+00 0.000000000D+00 2.645976732D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00    -2.472456805D+05-1.377221533D+02

Th(a)                    Alpha. Ref-Elm. Cox,1989 p239.  
 1 coda89 TH    1.00    0.00    0.00    0.00    0.00 1    232.0381000    0.000  
 200.000    1650.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0    6350.000  
 -1.453247151D+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

## Appendix D (continued)

Th(b)                      Beta. Ref-Elm. Cox,1989 p239.

1	coda89 TH	1.00	0.00	0.00	0.00	0.00	0.00	2	232.0381000	0.000
	1650.000	2023.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	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	0.00	3	232.0381000	0.000
	2023.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	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. Ref-Elm. Cox,1989 p230.

2	coda89 TI	1.00	0.00	0.00	0.00	0.00	1	47.8670000	0.000	
	200.000	900.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	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
	-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. Ref-Elm. Cox,1989 p230.

1	coda89 TI	1.00	0.00	0.00	0.00	0.00	2	47.8670000	0.000	
	1156.000	1944.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-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	47.8670000	0.000	
	1944.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	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			

TiB(cr)                      Crystal. Chase,1998. p258.

2	j 6/65 TI	1.00B	1.00	0.00	0.00	0.00	1	58.6780000	-160247.000	
	298.150	1100.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	5.892962460D+05	-7.628387170D+03	3.264504220D+01	-4.438679670D-02	4.037756110D-05					
	-1.901806786D-08	3.662438970D-12				1.808566462D+04	-1.924926707D+02			
	1100.000	4000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	9.736238960D+05	-2.744306202D+03	9.195602010D+00	-1.636706129D-03	5.676930840D-07					
	-9.258425040D-11	6.105669480D-15				-3.925082340D+03	-5.367424570D+01			

TiB2(cr)                      Crystal. Chase,1998 pp276-8.

2	j 6/65 TI	1.00B	2.00	0.00	0.00	0.00	1	69.4890000	-279491.000	
	200.000	2300.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	2.701885716D+05	-3.989107020D+03	1.904595810D+01	-1.467951261D-02	1.249126541D-05					
	-4.481179720D-09	5.932523160D-13				-1.510818691D+04	-1.130901290D+02			
	2300.000	3193.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	2.449855642D+10	-5.420046130D+07	4.984385950D+04	-2.437314870D+01	6.688502930D-03					
	-9.763538800D-07	5.923249200D-11				3.589528270D+08	-3.651406280D+05			

TiB2(L)                      Liquid. Chase,1998 pp276-8.

1	j 6/65 TI	1.00B	2.00	0.00	0.00	0.00	2	69.4890000	-279491.000	
	3193.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	0.000000000D+00	0.000000000D+00	1.308363331D+01	0.000000000D+00	0.000000000D+00					
	0.000000000D+00	0.000000000D+00				-3.298172270D+04	-7.649131141D+01			

TiC(cr)                      Chase,1998 p655-7

2	j 6/68 TI	1.00C	1.00	0.00	0.00	0.00	1	59.8777000	-184096.000	
	200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-2.936209453D+05	4.040416860D+03	-2.309999326D+01	8.695403030D-02	-1.254447445D-04					
	8.803423830D-08	-2.403516957D-11				-4.217890880D+04	1.253486677D+02			
	1000.000	3290.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	-3.586824960D+05	1.130360992D+03	4.571181220D+00	4.332844010D-04	4.730133770D-07					
	-1.025727737D-10	8.572441560D-15				-3.129994969D+04	-2.180975207D+01			

TiC(L)                      Chase,1998 p655-7

1	j 6/68 TI	1.00C	1.00	0.00	0.00	0.00	2	59.8777000	-184096.000	
	3290.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	0.000000000D+00	0.000000000D+00	7.548249987D+00	0.000000000D+00	0.000000000D+00					
	0.000000000D+00	0.000000000D+00				-1.766010062D+04	-4.062778302D+01			

TiCL2(cr)                      Chase,1998 p865.

2	j12/68 TI	1.00CL	2.00	0.00	0.00	0.00	1	118.7730000	-515470.000	
	200.000	800.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	6.275502170D+05	-1.149039253D+04	8.470916630D+01	-2.539508065D-01	4.582690050D-04					
	-4.167293950D-07	1.508542615D-10				-1.168917881D+04	-4.484122170D+02			
	800.000	2000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
	3.621030580D+06	-1.684661798D+04	4.010076440D+01	-2.963515568D-02	1.756075169D-05					
	-5.065847400D-09	5.988802280D-13				3.466967030D+04	-2.478759697D+02			

## Appendix D (continued)

TiCL3(cr) Chase,1998 p886.  
 1 j12/68 TI 1.00CL 3.00 0.00 0.00 0.00 1 154.2260000 -721740.000  
 298.150 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 20920.000  
 1.457928527D+05-1.355589207D+03 1.563840194D+01-4.771661650D-03 4.776265870D-06  
 -1.901286451D-09 3.011222662D-13 -8.308136940D+04-7.479338350D+01

TiCL4(L) Chase,1998 p904.  
 2 j12/67 TI 1.00CL 4.00 0.00 0.00 0.00 1 189.6790000 -804164.800  
 249.046 700.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26963.000  
 1.179781205D+06-1.710994382D+04 1.180652525D+02-3.089428313D-01 5.234695800D-04  
 -4.608788890D-07 1.654264781D-10 -2.053742284D+04-6.204956050D+02  
 700.000 2000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26963.000  
 0.000000000D+00 0.000000000D+00 1.714255083D+01 1.093131841D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.018779486D+05-6.764318260D+01

TiN(cr) Chase,1998 pp1612-4.  
 2 j 6/68 TI 1.00N 1.00 0.00 0.00 0.00 1 61.8737000 -337648.800  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5487.000  
 -5.479117220D+05 9.328691110D+03-6.386263890D+01 2.429925456D-01-4.304234520D-04  
 3.792645100D-07-1.317412256D-10 -8.424256140D+04 3.392988560D+02  
 800.000 3220.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5487.000  
 -3.656247060D+05 1.265730431D+03 3.831711190D+00 1.632900455D-03-1.062786626D-07  
 1.310931390D-11-5.770548410D-16 -5.027654400D+04-1.652632899D+01

TiN(L) Chase,1998 pp1612-4.  
 1 j 6/68 TI 1.00N 1.00 0.00 0.00 0.00 2 61.8737000 -337648.800  
 3220.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5487.000  
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.626039860D+04-3.958296649D+01

TiO(a) Alpha,monoclinic. Gurvich,1982 pt1 p98 pt2 p99.  
 2 tpis82 TI 1.000 1.00 0.00 0.00 0.00 1 63.8664000 -542000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6175.000  
 -1.126115023D+07 2.107240660D+05-1.601946203D+03 6.360717840D+00-1.380180278D-02  
 1.563169158D-05-7.238514780D-09 -1.014208223D+06 8.368056830D+03  
 500.000 1265.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6175.000  
 -2.066517895D+05 0.000000000D+00 8.243115270D+00-4.896702160D-03 3.806679150D-06  
 0.000000000D+00 0.000000000D+00 -6.815384410D+04-4.265310470D+01

TiO(b) Beta,cubic. Gurvich,1982 pt1 p98 pt2 p99.  
 1 tpis82 TI 1.000 1.00 0.00 0.00 0.00 2 63.8664000 -542000.000  
 1265.000 1810.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6175.000  
 -1.40082506D+05 0.000000000D+00 6.173304260D+00 1.455287203D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.756357790D+04-3.249519859D+01

TiO(c) Gamma,cubic. Gurvich,1982 pt1 p98 pt2 p99.  
 1 tpis82 TI 1.000 1.00 0.00 0.00 0.00 3 63.8664000 -542000.000  
 1810.000 2030.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6175.000  
 2.080459342D+05 0.000000000D+00 5.795530945D+00 1.404532558D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.627964090D+04-2.933709305D+01

TiO(L) Liquid. Gurvich,1982 pt1 p98 pt2 p99.  
 1 tpis82 TI 1.000 1.00 0.00 0.00 0.00 4 63.8664000 -542000.000  
 2030.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6175.000  
 0.000000000D+00 0.000000000D+00 8.419016875D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -6.314903830D+04-4.370051573D+01

TiO2(cr) Rutile,tetragonal. Gurvich,1982 pt1 p105 pt2 p105.  
 2 tpis82 TI 1.000 2.00 0.00 0.00 0.00 1 79.8658000 -944000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.000  
 1.712264157D+07-2.997059314D+05 2.143439285D+03-7.997230440D+00 1.661745261D-02  
 -1.817331921D-05 8.179403360D-09 1.253121023D+06-1.132509587D+04  
 500.000 2185.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.000  
 -1.244201863D+05 0.000000000D+00 7.600577340D+00 1.421666301D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.162831515D+05-3.834053430D+01

TiO2(L) Liquid. Gurvich,1982 pt1 p105 pt2 p105.  
 1 tpis82 TI 1.000 2.00 0.00 0.00 0.00 2 79.8658000 -944000.000  
 2185.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8680.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.143261561D+05-6.551584491D+01

Ti2O3(I) Hexagonal. Gurvich,1982 pt1 p109 pt2 p108.  
 2 tpis82 TI 2.000 3.00 0.00 0.00 0.00 1 143.7322000 -1520000.000  
 200.000 400.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14090.000  
 -1.771212920D+06 2.344459434D+04-1.110358342D+02 2.714352074D-01-1.921153675D-04  
 0.000000000D+00 0.000000000D+00 -2.995932792D+05 6.382146810D+02  
 400.000 464.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14090.000  
 0.000000000D+00 0.000000000D+00 5.692590423D+01-2.558542837D-01 3.734811793D-04  
 0.000000000D+00 0.000000000D+00 -1.917653868D+05-2.555304929D+02

## Appendix D (continued)

Ti2O3 (I') Hexagonal. Gurvich, 1982 pt1 p109 pt2 p108.  
 2 tpis82 TI 2.000 3.00 0.00 0.00 0.00 2 143.7322000 -1520000.000  
 464.000 580.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14090.000  
 0.000000000D+00 0.000000000D+00 9.288208205D+01 -2.728212486D-01 2.430399386D-04  
 0.000000000D+00 0.000000000D+00 -2.022790157D+05 -4.543828632D+02  
 580.000 2110.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14090.000  
 4.228751905D+05 0.000000000D+00 1.281963700D+01 4.013104801D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.858705711D+05 -6.399935229D+01

Ti2O3 (L) Liquid. Gurvich, 1982 pt1 p109 pt2 p108.  
 1 tpis82 TI 2.000 3.00 0.00 0.00 0.00 3 143.7322000 -1520000.000  
 2110.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 14090.000  
 0.000000000D+00 0.000000000D+00 2.044618384D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.821646342D+05 -1.087120898D+02

Ti3O5 (a) Alpha, monoclinic. Gurvich, 1982 pt1 p111 pt2 p110.  
 2 tpis82 TI 3.000 5.00 0.00 0.00 0.00 1 223.5980000 -2457000.000  
 200.000 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22630.000  
 0.000000000D+00 0.000000000D+00 4.315304530D+00 4.637018750D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.988551027D+05 -2.323385163D+01  
 298.150 448.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22630.000  
 -2.175887695D+07 0.000000000D+00 1.012212506D+03 -3.624156324D+00 3.726318087D-03  
 0.000000000D+00 0.000000000D+00 -5.421167010D+05 -4.959468179D+03

Ti3O5 (b) Beta, rhombic. Gurvich, 1982 pt1 p111 pt2 p110.  
 1 tpis82 TI 3.000 5.00 0.00 0.00 0.00 2 223.5980000 -2457000.000  
 448.000 2050.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22630.000  
 0.000000000D+00 0.000000000D+00 2.020131072D+01 5.124775844D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.004933224D+05 -9.863577455D+01

Ti3O5 (L) Liquid. Gurvich, 1982 pt1 p111 pt2 p110.  
 1 tpis82 TI 3.000 5.00 0.00 0.00 0.00 3 223.5980000 -2457000.000  
 2050.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22630.000  
 0.000000000D+00 0.000000000D+00 3.127063411D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.923316313D+05 -1.627424211D+02

Ti4O7 (cr) Triclinic. Gurvich, 1982 pt1 p112 pt2 p111.  
 2 tpis82 TI 4.000 7.00 0.00 0.00 0.00 1 303.4638000 -3403000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 35630.000  
 4.558528430D+06 -8.146955640D+04 5.758643730D+02 -1.933194123D+00 3.842536530D-03  
 -4.030781120D-06 1.748510017D-09 -4.239230760D+04 -3.066670887D+03  
 500.000 1960.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 35630.000  
 -4.675287930D+05 0.000000000D+00 2.961388604D+01 5.773820220D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.199386150D+05 -1.488468383D+02

Ti4O7 (L) Liquid. Gurvich, 1982 pt1 p112 pt2 p111.  
 1 tpis82 TI 4.000 7.00 0.00 0.00 0.00 2 303.4638000 -3403000.000  
 1960.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 35630.000  
 0.000000000D+00 0.000000000D+00 4.353834441D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.142527640D+05 -2.319810806D+02

U(a) Alpha. Ref-Elm. Cox, 1989 p234.  
 1 coda89 U 1.00 0.00 0.00 0.00 0.00 1 238.0289100 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 2 238.0289100 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 3 238.0289100 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 4 238.0289100 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

UF3 (cr) Hexagonal. Gurvich, 1982 pt1 p209 pt2 p236.  
 1 tpis82 U 1.00F 3.00 0.00 0.00 0.00 1 295.0241196 -1508700.000  
 298.150 1768.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18380.000  
 -1.245413139D+05 0.000000000D+00 1.281362341D+01 8.479152710D-05 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.856957321D+05 -5.889112439D+01

## Appendix D (continued)

UF3(L) Liquid. Gurvich,1982 pt1 p209 pt2 p236.  
 1 tps82 U 1.00F 3.00 0.00 0.00 0.00 2 295.0241196 -1508700.000  
 1768.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18380.000  
 0.000000000D+00 0.000000000D+00 1.611640373D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.869060867D+05-8.091478353D+01

UF4(cr) Monoclinic. Gurvich,1982 pt1 p212 pt2 p243.  
 2 tps82 U 1.00F 4.00 0.00 0.00 0.00 1 314.0225228 -1920500.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22550.000  
 -1.900846659D+06 3.555369140D+04-2.684351890D+02 1.162227739D+00-2.589319495D-03  
 2.991673531D-06-1.405949560D-09 -3.939232500D+05 1.401148993D+03  
 500.000 1309.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22550.000  
 -1.687548936D+05 0.000000000D+00 1.670280525D+01-3.858715240D-03 3.366874970D-06  
 0.000000000D+00 0.000000000D+00 -2.363858828D+05-7.687256170D+01

UF4(L) Liquid. Gurvich,1982 pt1 p212 pt2 p243.  
 1 tps82 U 1.00F 4.00 0.00 0.00 0.00 2 314.0225228 -1920500.000  
 1309.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 22550.000  
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.358206485D+05-9.894817389D+01

UF5(b) Beta,tetragonal. Gurvich,1982 pt1 p217 pt2 p250.  
 1 tps82 U 1.00F 5.00 0.00 0.00 0.00 1 333.0209260 -2083000.000  
 298.150 398.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26150.000  
 -2.315229641D+04 0.000000000D+00 1.505308190D+01 3.633166597D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.552530997D+05-6.539107895D+01

UF5(a) Alpha,tetragonal. Gurvich,1982 pt1 p217 pt2 p250.  
 1 tps82 U 1.00F 5.00 0.00 0.00 0.00 2 333.0209260 -2083000.000  
 398.000 621.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26150.000  
 -2.315229641D+04 0.000000000D+00 1.505308190D+01 3.633166597D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.542909264D+05-6.297355795D+01

UF5(L) Liquid. Gurvich,1982 pt1 p217 pt2 p250.  
 1 tps82 U 1.00F 5.00 0.00 0.00 0.00 3 333.0209260 -2083000.000  
 621.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 26150.000  
 0.000000000D+00 0.000000000D+00 2.008536883D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.524686368D+05-8.627305038D+01

UF6(cr) Rhombic. Gurvich,1982 pt1 p222 pt2 p532.  
 1 tps82 U 1.00F 6.00 0.00 0.00 0.00 1 352.0193292 -2197700.000  
 100.000 337.2107 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31565.000  
 1.490516238D+05-4.412150490D+03 5.041684430D+01-1.195638409D-01 2.070807828D-04  
 0.000000000D+00 0.000000000D+00 -2.502294955D+05-2.473731136D+02

UF6(L) Liquid. Gurvich,1982 pt1 p222 pt2 p532.  
 1 tps82 U 1.00F 6.00 0.00 0.00 0.00 2 352.0193292 -2197700.000  
 337.210 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 31565.000  
 0.000000000D+00 0.000000000D+00 1.750554152D+01 1.611640373D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.680142931D+05-7.051080543D+01

UO2(cr) Cubic. Gurvich,1982 pt1 p190 pt2 p209.  
 2 tps82 U 1.000 2.00 0.00 0.00 0.00 1 270.0277100 -1085000.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11280.000  
 -1.712140039D+07 3.206174610D+05-2.435851508D+03 9.665099460D+00-2.095506138D-02  
 2.371859464D-05-1.097936236D-08 -1.574556829D+06 1.272869884D+04  
 500.000 3123.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11280.000  
 -2.775509993D+05 0.000000000D+00 1.161094006D+01-3.430918270D-03 2.044412020D-06  
 0.000000000D+00 0.000000000D+00 -1.347529024D+05-5.751912860D+01

UO2(L) Liquid. Gurvich,1982 pt1 p190 pt2 p209.  
 1 tps82 U 1.000 2.00 0.00 0.00 0.00 2 270.0277100 -1085000.000  
 3123.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 11280.000  
 0.000000000D+00 0.000000000D+00 1.575558872D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.342007409D+05-8.859616713D+01

UO2F2(cr) Hexagonal. Gurvich,1982 pt1 p227 pt2 p262.  
 2 tps82 U 1.000 2.00F 2.00 0.00 0.00 1 308.0245164 -1653600.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19700.000  
 2.774535231D+06-5.047416500D+04 3.733097480D+02-1.349660046D+00 2.816624451D-03  
 -3.086048235D-06 1.391361959D-09 2.724906305D+04-1.962630228D+03  
 500.000 2100.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 19700.000  
 -1.227714401D+05 0.000000000D+00 1.277741930D+01 3.406816370D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -2.032540376D+05-5.821006900D+01

## Appendix D (continued)

UO3(c)                    Gamma, monoclinic. Gurvich, 1982 pt1 p195 pt2 p217.

2 tps82 U	1.000	3.00	0.00	0.00	0.00	0.00	1	286.0271100	-1223800.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.956676511D+06	3.951756640D+04	-3.223198540D+02	1.417862899D+00	-3.236211090D-03					
3.806716410D-06	-1.814492554D-09		-3.239008630D+05	1.660601808D+03					
500.000	3000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.090516805D+05	0.000000000D+00	1.271766576D+01	-2.508681376D-03	2.295592116D-06					
0.000000000D+00	0.000000000D+00		-1.515901509D+05	-6.143076620D+01					

U3O8(II)                    Rhombic. Gurvich, 1982 pt1 p199 pt2 p222.

2 tps82 U	3.000	8.00	0.00	0.00	0.00	0.00	1	842.0819300	-3574800.000
200.000	300.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.312654971D+05	0.000000000D+00	1.981648464D+01	3.463180280D-02	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-4.378350230D+05	-8.998750380D+01					
300.000	483.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.819324251D+06	0.000000000D+00	1.227600892D+02	-2.415563843D-01	0.000000000D+00					
3.622285580D-07	0.000000000D+00		-4.659833440D+05	-6.124926920D+02					

U3O8(I)                    Hexagonal. Gurvich, 1982 pt1 p199 pt2 p222.

1 tps82 U	3.000	8.00	0.00	0.00	0.00	0.00	2	842.0819300	-3574800.000
483.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-5.848811295D+04	0.000000000D+00	2.988522475D+01	6.597141623D-03	-4.626851131D-07					
0.000000000D+00	0.000000000D+00		-4.394086740D+05	-1.388063306D+02					

U4O9(III)                    Cubic. Gurvich, 1982 pt1 p201 pt2 p223.

1 tps82 U	4.000	9.00	0.00	0.00	0.00	0.00	1	1096.1102400	-4512000.000
298.150	348.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.274607283D+08	0.000000000D+00	6.797154853D+03	-2.205931654D+01	0.000000000D+00					
4.712462238D-05	0.000000000D+00		-2.109373967D+06	-3.324352924D+04					

U4O9(II)                    Cubic. Gurvich, 1982 pt1 p201 pt2 p223.

2 tps82 U	4.000	9.00	0.00	0.00	0.00	0.00	2	1096.1102400	-4512000.000
348.000	380.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.572378889D+07	0.000000000D+00	-1.352246013D+03	2.459469770D+00	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-3.013155679D+04	7.375484389D+03					
380.000	1398.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-7.968840016D+05	0.000000000D+00	4.574063896D+01	-1.083792070D-02	9.691491140D-06					
0.000000000D+00	0.000000000D+00		-5.582419360D+05	-2.211132773D+02					

U4O9(I)                    Gurvich, 1982 pt1 p201 pt2 p223.

1 tps82 U	4.000	9.00	0.00	0.00	0.00	0.00	3	1096.1102400	-4512000.000
1398.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.094590060D+05	0.000000000D+00	3.592971805D+01	1.009247689D-02	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-5.555228520D+05	-1.695188988D+02					

V(cr)                    Crystal. Ref-Elm. Chase, 1998 p1917.

3 j 6/73 V	1.00	0.00	0.00	0.00	0.00	0.00	1	50.9415000	0.000
200.000	600.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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
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
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	0.00	2	50.9415000	0.000
2190.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
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					

VCL2(cr)                    Pankratz, 1984.

1 g10/00 V	1.00CL	2.00	0.00	0.00	0.00	0.00	1	121.8475000	-451872.000
298.000	1300.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.844575327D+04	0.000000000D+00	8.648281619D+00	1.435173931D-03	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-5.711862150D+04	-3.824393774D+01					

VCL3(cr)                    Pankratz, 1984.

1 g 8/00 V	1.00CL	3.00	0.00	0.00	0.00	0.00	1	157.3005000	-581115.760
298.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-1.163436931D+05	0.000000000D+00	1.218941730D+01	1.091980165D-03	0.000000000D+00					
0.000000000D+00	0.000000000D+00		-7.396479110D+04	-5.467967609D+01					



## Appendix D (continued)

VN(cr) Chase,1998 p1635.

2 j12/73 V	1.00N	1.00	0.00	0.00	0.00	1	64.9482000	-217150.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
2.091900078D+05	-3.051142421D+03	1.689002455D+01	-2.016563261D-02	2.024805796D-05				
-9.052281300D-09	1.375923345D-12		-1.233229950D+04	-9.561817060D+01				
1000.000	3500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
8.212748990D+05	-2.203406736D+03	6.907596040D+00	1.164274622D-03	-3.307430080D-07				
1.061954757D-10	-1.105176783D-14		-1.341131421D+04	-3.925480780D+01				

VO(cr) Cubic Gurvich,1982 pt1 p60 pt2 p63.

2 tpi82 V	1.000	1.00	0.00	0.00	0.00	1	66.9409000	-430800.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-2.040260824D+07	3.783102280D+05	-2.848005957D+03	1.118080448D+01	-2.407270159D-02				
2.710471323D-05	-1.249526447D-08		-1.758506851D+06	1.490654242D+04				
500.000	2063.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-1.970015037D+05	0.000000000D+00	6.365723760D+00	1.576630310D-03	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-5.444168120D+04	-3.381741570D+01				

VO(L) Liquid Gurvich,1982 pt1 p60 pt2 p63.

1 tpi82 V	1.000	1.00	0.00	0.00	0.00	2	66.9409000	-430800.000
2063.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	8.419016875D+00	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-4.921350390D+04	-4.329727468D+01				

V2O3(cr) Hexagonal. Gurvich,1982 pt1 p65 pt2 p67.

2 tpi82 V	2.000	3.00	0.00	0.00	0.00	1	149.8812000	-1216800.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-2.445935804D+07	4.555627240D+05	-3.448966200D+03	1.365879117D+01	-2.955666350D-02				
3.340613030D-05	-1.544661718D-08		-2.200372063D+06	1.802928653D+04				
500.000	2230.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-4.148342860D+05	0.000000000D+00	1.735995875D+01	-2.248234102D-03	1.310940149D-06				
0.000000000D+00	0.000000000D+00		-1.528252156D+05	-8.926688900D+01				

V2O3(L) Liquid. Gurvich,1982 pt1 p65 pt2 p67.

1 tpi82 V	2.000	3.00	0.00	0.00	0.00	2	149.8812000	-1216800.000
2230.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	1.924346714D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.407455834D+05	-9.794985841D+01				

V2O4(II) Monoclinic. Gurvich,1982 pt1 p67 pt2 p68.

1 tpi82 V	2.000	4.00	0.00	0.00	0.00	1	165.8806000	-1432600.000
200.000	338.7007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-4.872822280D+05	0.000000000D+00	4.755837160D+01	-1.909710602D-01	3.188918050D-04				
0.000000000D+00	0.000000000D+00		-1.824442970D+05	-2.197380006D+02				

V2O4(I) Tetragonal. Gurvich,1982 pt1 p67 pt2 p68.

1 tpi82 V	2.000	4.00	0.00	0.00	0.00	2	165.8806000	-1432600.000
338.700	1818.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-3.456246971D+05	0.000000000D+00	1.740258897D+01	2.292498295D-03	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.776670154D+05	-8.737764367D+01				

V2O4(L) Liquid. Gurvich,1982 pt1 p67 pt2 p68.

1 tpi82 V	2.000	4.00	0.00	0.00	0.00	3	165.8806000	-1432600.000
1818.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	2.164890054D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.679377747D+05	-1.076187785D+02				

V2O5(cr) Rhombic. Gurvich,1982 pt1 p68 pt2 p69.

2 tpi82 V	2.000	5.00	0.00	0.00	0.00	1	181.8800000	-1551000.000
200.000	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-1.149585895D+07	2.200852292D+05	-1.711429444D+03	6.997610220D+00	-1.543892990D-02				
1.771425949D-05	-8.283987620D-09		-1.174509299D+06	8.899979010D+03				
500.000	954.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
-4.708328420D+05	0.000000000D+00	2.297387367D+01	-1.118831481D-02	1.146815480D-05				
0.000000000D+00	0.000000000D+00		-1.945738450D+05	-1.150219507D+02				

V2O5(L) Liquid. Gurvich,1982 pt1 p68 pt2 p69.

1 tpi82 V	2.000	5.00	0.00	0.00	0.00	2	181.8800000	-1551000.000
954.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0 0.0
0.000000000D+00	0.000000000D+00	2.285161723D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-1.880385445D+05	-1.113109611D+02				

## Appendix D (continued)

W(cr) Crystal. Ref-Elm. Chase,1998 pp1925-8.

4 j 6/66 W	1.00	0.00	0.00	0.00	0.00	1	183.8400000	0.000
200.000	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-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
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
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
-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 pp1925-8.

1 j 6/66 W	1.00	0.00	0.00	0.00	0.00	2	183.8400000	0.000
3680.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+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				

WC(cr) Hf:Wagman,1982 p203. Barin,1989 pt2 p1642.

1 bar 89 W	1.00C	1.00	0.00	0.00	0.00	1	195.8507000	-40540.000
298.150	2500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.119754391D+05	-5.553268210D-01	5.217965240D+00	1.037888263D-03	-1.229060652D-07				
2.880427321D-13	-7.236307119D-17		-6.848998700D+03	-2.677066218D+01				

WCL6(I) Alpha1. Chase,1998 pp931-4.

1 j12/66 W	1.00CL	6.00	0.00	0.00	0.00	1	396.5580000	-593710.000
298.150	450.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.661826519D+02	0.000000000D+00	1.508873100D+01	2.015651227D-02	-2.754798370D-08				
0.000000000D+00	0.000000000D+00		-7.680028810D+04	-6.329365920D+01				

WCL6(II) Alpha2. Chase,1998 pp931-4.

1 j12/66 W	1.00CL	6.00	0.00	0.00	0.00	2	396.5580000	-593710.000
450.000	503.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-9.897046360D+03	0.000000000D+00	1.522857952D+01	1.994376611D-02	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-7.636166220D+04	-6.296167010D+01				

WCL6(III) Beta. Chase,1998 pp931-4.

1 j12/66 W	1.00CL	6.00	0.00	0.00	0.00	3	396.5580000	-593710.000
503.000	555.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.264474996D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-7.565217840D+04	-9.527165358D+01				

WCL6(L) Liquid. Chase,1998 pp931-4.

1 j12/66 W	1.00CL	6.00	0.00	0.00	0.00	4	396.5580000	-593710.000
555.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.415439996D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-7.568493560D+04	-1.033604557D+02				

WOCL4(cr) Crystal. Chase,1998 pp897-9.

1 j 3/67 W	1.000	1.00CL	4.00	0.00	0.00	1	341.6514000	-671114.000
298.150	484.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
1.295153216D+03	0.000000000D+00	1.378522135D+01	1.276179773D-02	-1.713279395D-07				
0.000000000D+00	0.000000000D+00		-8.538742740D+04	-6.154983780D+01				

WOCL4(L) Liquid. Chase,1998 pp897-9.

1 j 3/67 W	1.000	1.00CL	4.00	0.00	0.00	2	341.6514000	-671114.000
484.000	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
0.000000000D+00	0.000000000D+00	2.188992496D+01	0.000000000D+00	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-8.236656270D+04	-9.422321377D+01				

WO2(cr) Gurvich,1982 pt1 p46 pt2 p49.

2 tpis82 W	1.000	2.00	0.00	0.00	0.00	1	215.8388000	-588100.000
100.000	298.1507	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.733842408D+04	0.000000000D+00	2.558979845D+00	1.457260175D-02	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-7.220058630D+04	-1.293182268D+01				
298.150	6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-1.555714047D+05	0.000000000D+00	7.983272616D+00	1.595163155D-03	0.000000000D+00				
0.000000000D+00	0.000000000D+00		-7.370467050D+04	-4.074555290D+01				

WO2CL2(cr) Chase,1998 p848.

1 j 3/67 W	1.000	2.00CL	2.00	0.00	0.00	1	286.7448000	-780316.000
298.150	1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0
-3.819410020D+05	2.367029691D+03	9.834455770D+00	-2.508443012D-02	1.017169638D-04				
-1.040117941D-07	3.468311980D-11		-1.111440350D+05	-2.227929881D+01				

## Appendix D (continued)

WO3(III) Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 0.00 1 231.8382000 -841300.000  
 100.000 325.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13280.000  
 -2.841140443D+05 7.257714840D+03-6.708405120D+01 3.092936300D-01-4.127635650D-04  
 0.000000000D+00 0.000000000D+00 -1.335884160D+05 3.409113710D+02

WO3(III,II) Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 0.00 2 231.8382000 -841300.000  
 325.000 1013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13280.000  
 -5.186114395D+04 0.000000000D+00 8.548308920D+00 4.317151582D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.040935177D+05-4.044670662D+01

WO3(I) Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 0.00 3 231.8382000 -841300.000  
 1013.000 1747.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13280.000  
 0.000000000D+00 0.000000000D+00 9.737555190D+00 1.958624140D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.039166330D+05-4.614390358D+01

WO3(L) Liquid. Gurvich,1982 pt1 p49 pt2 p51.  
 1 tpis82 W 1.000 3.00 0.00 0.00 0.00 0.00 4 231.8382000 -841300.000  
 1747.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 13280.000  
 0.000000000D+00 0.000000000D+00 1.551504538D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.022412072D+05-8.082927535D+01

Zn(cr) Crystal. Ref-Elm. Cox,1989 p221.  
 1 coda89 ZN 1.00 0.00 0.00 0.00 0.00 0.00 1 65.3900000 0.000  
 200.000 692.7307 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5657.000  
 3.702080380D+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 0.00 2 65.3900000 0.000  
 692.730 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5657.000  
 0.000000000D+00 0.000000000D+00 3.776530427D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.317345880D+02-1.567077937D+01

ZnSO4(a) Alpha. Chase,1998 p1788.  
 1 j 3/79 ZN 1.00S 1.000 4.00 0.00 0.00 0.00 1 161.4526000 -980143.840  
 200.000 540.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17238.080  
 4.103530390D+05-7.357987120D+03 5.215317850D+01-1.152180317D-01 1.922132213D-04  
 -1.099361720D-07 0.000000000D+00 -8.649370210D+04-2.794432413D+02

ZnSO4(a') Alpha'.Chase,1998 p1788.  
 1 j 3/79 ZN 1.00S 1.000 4.00 0.00 0.00 0.00 2 161.4526000 -980143.840  
 540.000 1013.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17238.080  
 -3.253792010D+06 3.252313710D+04-1.146490609D+02 2.718567520D-01-3.079986965D-04  
 1.830520033D-07-4.445112450D-11 -2.895173465D+05 6.881710230D+02

ZnSO4(b) Beta. Chase,1998 p1788.  
 1 j 3/79 ZN 1.00S 1.000 4.00 0.00 0.00 0.00 3 161.4526000 -980143.840  
 1013.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 17238.080  
 0.000000000D+00 0.000000000D+00 1.746161830D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.211366813D+05-8.514209609D+01

Zr(a) Alpha. Ref-Elm. Chase,1998 pp1943-7.  
 1 j 6/79 ZR 1.00 0.00 0.00 0.00 0.00 0.00 1 91.2240000 0.000  
 200.000 1135.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5497.000  
 -1.153699220D+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 pp1943-7.  
 1 j 6/79 ZR 1.00 0.00 0.00 0.00 0.00 0.00 2 91.2240000 0.000  
 1135.000 2125.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5497.000  
 -1.065463955D+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 pp1943-7.  
 1 j 6/79 ZR 1.00 0.00 0.00 0.00 0.00 0.00 3 91.2240000 0.000  
 2125.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5497.000  
 0.000000000D+00 0.000000000D+00 5.032166658D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.100795852D+03-2.548066000D+01

ZrC(cr) Crystal. Chase,1998 pp658-60.  
 2 j12/64 ZR 1.00C 1.00 0.00 0.00 0.00 0.00 1 103.2347000 -196648.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5862.000  
 -1.329596558D+05 1.766908163D+03-9.907099000D+00 5.427909170D-02-8.887722520D-05  
 7.332246190D-08-2.420411623D-11 -3.297124410D+04 5.279964170D+01  
 800.000 3805.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5862.000  
 8.297591180D+05-4.224196050D+03 1.308509211D+01-5.018095870D-03 2.155019459D-06  
 -4.233046770D-10 3.266859200D-14 -7.112782350D+02-7.921945570D+01

## Appendix D (continued)

ZrC(L) Liquid. Chase,1998 pp658-60.  
 1 j12/64 ZR 1.00C 1.00 0.00 0.00 0.00 2 103.2347000 -196648.000  
 3805.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 5862.000  
 0.000000000D+00 0.000000000D+00 7.548249987D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.885005134D+04-3.953387107D+01

ZrN(cr) Chase,1998 pp1617-9 6/61.  
 2 g11/00 ZR 1.00N 1.00 0.00 0.00 0.00 1 105.2307000 -371238.000  
 200.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6590.000  
 2.548624207D+05-4.476456170D+03 2.958601499D+01-6.635810940D-02 1.033814686D-04  
 -8.272994600D-08 2.689947231D-11 -2.492379728D+04-1.616084405D+02  
 800.000 3225.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6590.000  
 2.174089790D+05-1.074470994D+03 7.053124150D+00-1.447713245D-04 3.458043010D-07  
 -5.893486000D-11 3.787112980D-15 -3.999164210D+04-3.811591880D+01

ZrN(L) Chase,1998 pp1617-9 6/61.  
 1 g11/00 ZR 1.00N 1.00 0.00 0.00 0.00 2 105.2307000 -371238.000  
 3225.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 6590.000  
 0.000000000D+00 0.000000000D+00 7.045033321D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -3.882762780D+04-3.444078302D+01

ZrO2(III) Monoclinic. Gurvich,1982 pt1 p123 pt2 p122.  
 2 tps82 ZR 1.00O 2.00 0.00 0.00 0.00 1 123.2228000 -1100300.000  
 200.000 500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8751.000  
 -4.214621830D+06 7.918732350D+04-6.071267910D+02 2.463358622D+00-5.388665930D-03  
 6.144154000D-06-2.860860736D-09 -4.893051030D+05 3.163542730D+03  
 500.000 1445.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8751.000  
 -1.616911113D+05 0.000000000D+00 8.218464380D+00 1.091902502D-03 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.353760676D+05-4.200007680D+01

ZrO2(II) Tetragonal. Gurvich,1982 pt1 p123 pt2 p122.  
 1 tps82 ZR 1.00O 2.00 0.00 0.00 0.00 2 123.2228000 -1100300.000  
 1445.000 2620.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8751.000  
 0.000000000D+00 0.000000000D+00 9.393217399D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.348114469D+05-4.823174581D+01

ZrO2(I) Cubic. Gurvich,1982 pt1 p123 pt2 p122.  
 1 tps82 ZR 1.00O 2.00 0.00 0.00 0.00 3 123.2228000 -1100300.000  
 2620.000 2983.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8751.000  
 0.000000000D+00 0.000000000D+00 9.621733572D+00 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.338466275D+05-4.943361269D+01

ZrO2(L) Liquid. Gurvich,1982 pt1 p123 pt2 p122.  
 1 tps82 ZR 1.00O 2.00 0.00 0.00 0.00 4 123.2228000 -1100300.000  
 2983.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8751.000  
 0.000000000D+00 0.000000000D+00 1.202716696D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -1.301975851D+05-6.505001424D+01

END PRODUCTS

Air Mole%:N2 78.084,O2 20.9476,Ar .9365,CO2 .0319.Gordon,1982.Reac  
 2 g 9/95 N 1.56170 .41959AR.00937C .00032 .00000 0 28.9651159 -125.530  
 200.000 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8649.264  
 1.009950160D+04-1.968275610D+02 5.009155110D+00-5.761013730D-03 1.066859930D-05  
 -7.940297970D-09 2.185231910D-12 -1.767967310D+02-3.921504225D+00  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 8649.264  
 2.415214430D+05-1.257874600D+03 5.144558670D+00-2.138541790D-04 7.065227840D-08  
 -1.071483490D-11 6.577800150D-16 6.462263190D+03-8.147411905D+00

B2H6(L) Diborane. McBride,1996 pp84,92.  
 0 g 6/96 B 2.00H 6.00 0.00 0.00 0.00 1 27.6696400 16445.000  
 180.590 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.000

B5H9(L) Pentaborane. Chase,1998 p302.  
 0 j 3/65 B 5.00H 9.00 0.00 0.00 0.00 1 63.1264600 42840.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.000

(CH2)x(cr) Ethylene polymer. McBride,1996 pp84,92.  
 0 g 6/96 C 1.00H 2.00 0.00 0.00 0.00 1 14.0265800 -25600.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.000

CH3NO2(L) Nitromethane. McBride,1996 pp85,93.  
 0 g 6/96 C 1.00H 3.00N 1.00O 2.00 0.00 1 61.0400200 -113100.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.000

CH4(L) Methane. McBride,1996 pp85,93.  
 0 g 6/96 C 1.00H 4.00 0.00 0.00 0.00 1 16.0424600 -89233.000  
 111.643 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.000

CH3OH(L) MeOH. TRC(12/87) p5000 (12/84)tc,uc,vc5031,5033. React.  
 1 n12/84 C 1.00H 4.00O 1.00 0.00 0.00 1 32.0418600 -238910.000  
 175.610 390.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0 18995.000  
 -1.302004763D+06 3.166984180D+04-3.031242152D+02 1.602231130D+00-4.594507340D-03  
 6.990178310D-06-4.207388950D-09 -1.656168201D+05 1.514346642D+03

## Appendix D (continued)

CH6N2(L) Monomethyl Hydrazine. TRC(12/93) p9220.									
0 n12/93 C	1.00H	6.00N	2.00	0.00	0.00	1	46.0717400	54200.000	
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C2H2(L),acetylene Acetylene. McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	2.00	0.00	0.00	0.00	1	26.0372800	207599.000	
192.350	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
CH3CN(L) Ethanenitrile (Acetonitrile). McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	3.00N	1.00	0.00	0.00	1	41.0519200	31380.000	
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C2H4(L) Ethylene. McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	4.00	0.00	0.00	0.00	1	28.0531600	33945.000	
169.420	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C2H4O(L),ethylene Ethylene oxide (Oxirane). McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	4.00O	1.00	0.00	0.00	1	44.0525600	-78841.000	
283.650	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C2H6(L) Ethane. McBride,1996 pp84,92.									
0 g 6/96 C	2.00H	6.00	0.00	0.00	0.00	1	30.0690400	-103819.000	
184.559	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C2H5OH(L) Ethanol. TRC(12/87) p5000 (12/84) tc,uc,vc5031-3. React.									
1 n12/84 C	2.00H	6.00O	1.00	0.00	0.00	1	46.0684400	-277510.000	
159.000	390.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
4.501115940D+05	-1.020828990D+04	1.014266780D+02	-3.874672610D-01	7.121392610D-04	-1.857071450D-07	-2.037622570D-10	7.448557900D+03	-5.044255520D+02	
C2H8N2(L),UDMH Unsymmetrical Dimethyl Hydrazine. McBride,1996 pp85,93.									
0 g 6/96 C	2.00H	8.00N	2.00	0.00	0.00	1	60.0983200	48900.000	
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C2N2(L) Cyanogen. McBride,1996 pp84,92.									
0 g 6/96 C	2.00N	2.00	0.00	0.00	0.00	1	52.0348000	283209.000	
252.050	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C3H6(L),propylene Propylene. McBride,1996 pp85,93.									
0 g 6/96 C	3.00H	6.00	0.00	0.00	0.00	1	42.0797400	-2704.000	
225.460	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C3H7NO3(L) Propyl Nitrate. McBride,1996 pp85,93.									
0 g 6/96 C	3.00H	7.00N	1.00O	3.00	0.00	1	105.0925800	-214500.000	
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C3H8(L) Propane. McBride,1996 pp85,93.									
0 g 6/96 C	3.00H	8.00	0.00	0.00	0.00	1	44.0956200	-128228.000	
231.076	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C4H8(L),1-buten 1-Butene. McBride,1996 pp84,92.									
0 g 6/96 C	4.00H	8.00	0.00	0.00	0.00	1	56.1063200	-25173.000	
266.920	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C4H10(L),n-buta n-Butane. McBride,1996 pp84,92.									
0 g 6/96 C	4.00H	10.00	0.00	0.00	0.00	1	58.1222000	-150664.000	
272.638	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C4H10(L),isobut Isobutane(2-methyl propane). McBride,1996 pp84,92.									
0 g 6/96 C	4.00H	10.00	0.00	0.00	0.00	1	58.1222000	-159664.000	
261.361	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C5H12(L),n-pent n-Pentane. McBride,1996 pp85,93.									
0 g 6/96 C	5.00H	12.00	0.00	0.00	0.00	1	72.1487800	-173490.000	
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.000	
C6H6(L) TRC(10/86) tc,uc,vc3201 (4/83) p3200. React.									
1 n10/86 C	6.00H	6.00	0.00	0.00	0.00	1	78.1118400	49080.000	
278.680	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-2.291003940D+06	3.692058160D+04	-1.820019971D+02	2.634137216D-01	9.742585920D-04	-3.307909150D-06	2.888191394D-09	-1.730169095D+05	1.070458659D+03	
C6H5NH2(L) Aniline. TRC(12/88) tc,uc,vc9370. TRC(6/95) p9370. React.									
1 n12/88 C	6.00H	7.00N	1.00	0.00	0.00	1	93.1264800	31500.000	
267.130	460.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
6.257653490D+07	-8.930118090D+05	5.055201440D+03	-1.397470822D+01	1.889729680D-02	-9.205910240D-06	-1.289458554D-09	4.267459270D+06	-2.801220752D+04	
C6H14(L),n-hexa n-hexane. TRC(4/85) p,tc,uc,vc1440,1441. React.									
1 n 4/85 C	6.00H	14.00	0.00	0.00	0.00	1	86.1753600	-198660.000	
177.860	300.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
7.721016130D+06	-2.249298616D+05	2.717090647D+03	-1.698251992D+01	5.907215180D-02	-1.074528475D-04	8.024238270D-08	8.808691730D+05	-1.292771483D+04	
C7H8(L) TRC(10/86) tc uc vc3200-1 (4/83) p-3200. React.									
1 n10/86 C	7.00H	8.00	0.00	0.00	0.00	1	92.1384200	12180.000	
178.150	500.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0
-3.713549510D+06	7.772529030D+04	-6.312269860D+02	2.724391982D+00	-6.103535080D-03	7.022421900D-06	-3.113715680D-09	-3.452115500D+05	3.265980710D+03	

## Appendix D (continued)

C7H16(L), n-hept										TRC(10/84)	p-1010	(10/75)	tc,uc,vcl460.	React.
1	n10/75	C	7.00H	16.00	0.00	0.00	0.00	1	100.2019400	-224350.000				
	182.580		380.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	52640.000		
1.759947367D+06-3.749396790D+04										3.963064900D+02-2.117827431D+00	6.828248670D-03			
-1.131862116D-05										7.736860130D-09	1.269072572D+05-1.921686840D+03			
C8H18(L), n-octa										TRC(10/76)	tc,uc,vcl491,1492.	Hf:(10/84)	p1010.	
1	n10/84	C	8.00H	18.00	0.00	0.00	0.00	1	114.2285200	-250260.000				
	216.370		400.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	61490.000		
-1.683314826D+07										3.532615080D+05-2.967857531D+03	1.316703807D+01-3.186822410D-02			
4.075748010D-05-2.153277285D-08										-1.588494258D+06	1.521639569D+04			
C8H18(L), isoact										TRC(10/76)	tc,uc,vcl491,1492.	Hf:(10/82)	p1490.	
1	n10/82	C	8.00H	18.00	0.00	0.00	0.00	1	114.2285200	-259160.000				
	165.790		380.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	50190.000		
1.419157943D+05-2.937251288D+03										4.168834760D+01-8.436942210D-02	2.894147919D-04			
-2.200563712D-07										7.234225570D-11	-2.479398829D+04-1.930220201D+02			
CLF3(L)										Chlorine Trifluoride. McBride,1996 pp84,92.				
0	g	6/96	CL	1.00F	3.00	0.00	0.00	0.00	1	92.4482096	-193386.000			
	284.890		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
CLO3F										Hf:Wagman,1982 p49. Chase,1998 p755.				
2	g	5/95	CL	1.00O	3.00F	1.00	0.00	0.00	0	102.4496032	-23800.000			
	200.000		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13298.823		
4.461077310D+04-5.892352210D+02										3.558850810D+00	2.809585831D-02-3.610880350D-05			
2.273331859D-08-5.716733040D-12										-1.388667752D+03	4.590741392D+00			
	1000.000		6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	13298.823		
-3.910495440D+05-1.193220687D+03										1.388657545D+01-3.541312060D-04	7.825464770D-08			
-8.978325430D-12										4.163869660D-16	-1.275082535D+03-5.106452991D+01			
CLO3F(L)										Perchloryl Fluoride. McBride,1996 pp85,93.				
0	g	6/96	CL	1.00O	3.00F	1.00	0.00	0.00	1	102.4496032	-47436.000			
	226.400		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
CL2(L)										Chlorine. McBride,1996 pp84,92.				
0	g	6/96	CL	2.00	0.00	0.00	0.00	0.00	1	70.9060000	-22550.000			
	239.120		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
F2(L)										Fluorine. McBride,1996 pp84,92.				
0	g	6/96	F	2.00	0.00	0.00	0.00	0.00	1	37.9968064	-13091.000			
	85.020		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
F2O(L)										Oxygen Difluoride. McBride,1996 pp85,93.				
0	g	6/96	F	2.00O	1.00	0.00	0.00	0.00	1	53.9962064	6672.000			
	128.400		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
HNO3(L)										Nitric Acid. McBride,1996 pp85,93.				
0	g	6/96	H	1.00N	1.00O	3.00	0.00	0.00	1	63.0128400	-173013.000			
	298.150		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
H2(L)										Hydrogen. McBride,1996 pp84,92.				
0	g	6/96	H	2.00	0.00	0.00	0.00	0.00	1	2.0158800	-9012.000			
	20.270		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
H2O2(L)										Gurvich, 1989 v1 pt1 p126 pt2 p303.				
1	tpis89	H	2.00O	2.00	0.00	0.00	0.00	1	34.0146800	-187780.000				
	272.740		6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22949.000		
0.000000000D+00										0.000000000D+00	1.074386825D+01	0.000000000D+00	0.000000000D+00	
0.000000000D+00										0.000000000D+00	-2.578789845D+04-4.803221291D+01			
IRFNA										Inhibited Red Fuming Nitric Acid. McBride,1996 pp84,93.				
0	g	6/96	H	1.57N	1.63O	4.70F	0.02	0.00	1	99.9905349	-270496.000			
	298.150		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
JP-4										McBride,1996 pp85,93. Hcomb = 18640.BTU/#				
0	g	6/96	C	1.00H	1.94	0.00	0.00	0.00	1	13.9661036	-22723.000			
	298.150		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
JP-5										Or ASTM1(L). McBride,1996 pp85,93. Hcomb = 18600.BTU/#				
0	g	6/96	C	1.00H	1.92	0.00	0.00	0.00	1	13.9459448	-22183.000			
	298.150		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
JP-10(L)										Exo-tetrahydrodicyclopentadiene. Smith,1979.				
0	g	6/01	C	10.00H	16.00	0.00	0.00	0.00	0	136.2340400	-122800.400			
	298.150		0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000		
JP-10(g)										Exo-tetrahydrodicyclopentadiene.Pri.Com.R.Jaffe 12/00.				
2	g	6/01	C	10.00H	16.00	0.00	0.00	0.00	0	136.2340400	-86855.900			
	200.000		1000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22997.434		
-7.310769440D+05										1.521764245D+04-1.139312644D+02	4.281501620D-01-5.218740440D-04			
3.357233400D-07-8.805750980D-11										-8.067482120D+04	6.320148610D+02			
	1000.000		6000.0007	-2.0	-1.0	0.0	1.0	2.0	3.0	4.0	0.0	22997.434		
1.220329594D+07-5.794846240D+04										1.092281156D+02-1.082406215D-02	2.034992622D-06			
-2.052060369D-10										8.575760210D-15	3.257334050D+05-7.092350760D+02			

## Appendix D (continued)

Jet-A(L) McBride,1996. Faith,1971. Gracia-Salcedo,1988. React.  
 1 g 2/96 C 12.00H 23.00 0.00 0.00 0.00 1 167.3110200 -303403.000  
 220.000 550.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 -4.218262130D+05-5.576600450D+03 1.522120958D+02-8.610197550D-01 3.071662234D-03  
 -4.702789540D-06 2.743019833D-09 -3.238369150D+04-6.781094910D+02

Jet-A(g) McBride,1996. Faith,1971. Gracia-Salcedo,1988. React.  
 2 g 8/01 C 12.00H 23.00 0.00 0.00 0.00 0 167.3110200 -249657.000  
 273.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 -6.068695590D+05 8.328259590D+03-4.312321270D+01 2.572390455D-01-2.629316040D-04  
 1.644988940D-07-4.645335140D-11 -7.606962760D+04 2.794305937D+02  
 1000.000 6000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 1.858356102D+07-7.677219890D+04 1.419826133D+02-7.437524530D-03 5.856202550D-07  
 1.223955647D-11-3.149201922D-15 4.221989520D+05-8.986061040D+02

LiClO4(cr) Lithium Perchlorate. Chase,1998 p782.  
 0 g 6/96 LI 1.00CL 1.000 4.00 0.00 0.00 1 106.3916000 -380700.000  
 298.150 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

NF3(L) Nitrogen trifluoride. McBride,1996 pp85,93.  
 0 g 6/96 N 1.00F 3.00 0.00 0.00 0.00 1 71.0019096 -150387.000  
 144.090 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

NH3(L) Ammonia. McBride,1996 pp84,92.  
 0 g 6/96 N 1.00H 3.00 0.00 0.00 0.00 1 17.0305200 -71555.000  
 239.720 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

NH4ClO4(I) Ammonium Perchlorate. Chase,1998 p766. React.  
 1 j12/62 N 1.00H 4.00CL 1.000 4.00 0.00 1 117.4890600 -295767.000  
 100.000 513.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 -3.075344900D+03-2.136506130D+02 1.021583093D+01 1.659463617D-02 1.665266832D-05  
 -2.306096672D-08 1.543657693D-11 -3.825767260D+04-4.230254380D+01

NH4ClO4(II) Ammonium Perchlorate. Chase,1998 p766. React.  
 2 j12/62 N 1.00H 4.00CL 1.000 4.00 0.00 2 117.4890600 -295767.000  
 513.150 1000.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 9.739327490D+06-7.095035120D+04 2.133435041D+02-2.657628679D-01 2.034168863D-04  
 -5.628229760D-08 0.000000000D+00 3.485366440D+05-1.304962218D+03  
 1000.000 1500.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 4.174684580D+06-1.716642636D+04 1.925955165D+01 3.499518910D-02-6.264443390D-06  
 -1.494354361D-09 0.000000000D+00 7.134752510D+04-1.274562074D+02

NH4NO3(IV) Rhombic(IV). Gurvich,1989 pt1 p370 pt2 p322. React.  
 2 tpis89 N 2.00H 4.000 3.00 0.00 0.00 1 80.0433600 -365600.000  
 256.200 298.1507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 -1.046561904D+07 1.560375249D+05-9.143153600D+02 2.670225944D+00-3.549932910D-03  
 1.692615192D-06 0.000000000D+00 -7.861735160D+05 5.038726210D+03  
 298.150 305.3807 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000000000D+00 0.000000000D+00 5.865649329D+00 3.643028874D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.733937230D+04-2.614362444D+01

NH4NO3(III) Rhombic(III). Gurvich,1989 pt1 p370 pt2 p322. React.  
 1 tpis89 N 2.00H 4.000 3.00 0.00 0.00 2 80.0433600 -365600.000  
 305.380 357.2507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000000000D+00 0.000000000D+00 7.233138213D+00 2.333270391D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.694179380D+04-2.929851693D+01

NH4NO3(II) Tetragonal(II). Gurvich,1989 pt1 p370 pt2 p322. React.  
 1 tpis89 N 2.00H 4.000 3.00 0.00 0.00 3 80.0433600 -365600.000  
 357.250 399.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000000000D+00 0.000000000D+00 6.023205216D+01-1.767993544D-01 0.000000000D+00  
 4.528829721D-07 0.000000000D+00 -5.478633510D+04-2.757806209D+02

NH4NO3(I) Cubic(I). Gurvich,1989 pt1 p370 pt2 p322. React.  
 1 tpis89 N 2.00H 4.000 3.00 0.00 0.00 4 80.0433600 -365600.000  
 399.000 442.8507 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000000000D+00 0.000000000D+00 1.295325882D+01 1.563531705D-02 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.783701280D+04-5.848510823D+01

NH4NO3(L) Liquid Gurvich,1989 pt1 p370 pt2 p322. React.  
 1 tpis89 N 2.00H 4.000 3.00 0.00 0.00 5 80.0433600 -365600.000  
 442.850 900.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 0.000000000D+00 0.000000000D+00 1.936373881D+01 0.000000000D+00 0.000000000D+00  
 0.000000000D+00 0.000000000D+00 -4.843793300D+04-8.903005276D+01

N2(L) Nitrogen. McBride,1996 pp85,93.  
 0 g 6/96 N 2.00 0.00 0.00 0.00 0.00 1 28.0134000 -12107.000  
 77.352 0.0000 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0

N2H4(L) Hydrazine.Hf:Gurvich,1989 pt1 p360. Chase,1998(12/65). React.  
 1 g11/99 N 2.00H 4.00 0.00 0.00 0.00 1 32.0451600 50380.000  
 100.000 800.0007 -2.0 -1.0 0.0 1.0 2.0 3.0 4.0 0.0  
 2.080965738D+04-7.418167630D+02 1.916569184D+01-4.539330120D-02 1.342024252D-04  
 -1.470873931D-07 6.056288260D-11 5.735408180D+03-8.820213940D+01

## Appendix D (concluded)

N2O4 (L)	Dinitrogen tetroxide. McBride,1996 pp85,93.										
0 g 6/96 N	2.000	4.00	0.00	0.00	0.00	1	92.0110000				-17549.000
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000
O2 (L)	Oxygen. McBride,1996 pp85,93.										
0 g 6/96 O	2.00	0.00	0.00	0.00	0.00	1	31.9988000				-12979.000
90.170	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000
O3 (L)	Ozone. McBride,1996 pp85,93.										
0 g 6/96 O	3.00	0.00	0.00	0.00	0.00	1	47.9982000				122527.000
161.850	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000
RP-1	Mehta et.al. AIAA 95-2962 1995. Hcomb(high) = 19923.BTU/#										
0 gll/00 C	1.00H	1.95	0.00	0.00	0.00	1	13.9761830				-24717.700
298.150	0.0000	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.000
END REACTANTS											



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Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)		2. REPORT DATE September 2002		3. REPORT TYPE AND DATES COVERED Technical Paper
4. TITLE AND SUBTITLE  NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species			5. FUNDING NUMBERS  WU-708-87-13-00	
6. AUTHOR(S)  Bonnie J. McBride, Michael J. Zehe, and Sanford Gordon				
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  National Aeronautics and Space Administration John H. Glenn Research Center at Lewis Field Cleveland, Ohio 44135-3191			8. PERFORMING ORGANIZATION REPORT NUMBER  E-13336	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)  National Aeronautics and Space Administration Washington, DC 20546-0001			10. SPONSORING/MONITORING AGENCY REPORT NUMBER  NASA TP-2002-211556	
11. SUPPLEMENTARY NOTES  Responsible person, Bonnie J. McBride, organization code 5830, 216-433-5870.				
12a. DISTRIBUTION/AVAILABILITY STATEMENT  Unclassified - Unlimited Subject Categories: 77, 61, and 28 Available electronically at <a href="http://gltrs.grc.nasa.gov/GLTRS">http://gltrs.grc.nasa.gov/GLTRS</a> This publication is available from the NASA Center for AeroSpace Information, 301-621-0390.			12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words)  This report documents the library of thermodynamic data used with the NASA Glenn computer program CEA (Chemical Equilibrium with Applications). This library, containing data for over 2000 solid, liquid, and gaseous chemical species for temperatures ranging from 200 to 20 000 K, is available for use with other computer codes as well. The data are expressed as least-squares coefficients to a seven-term functional form for $C_p^o(T)/R$ with integration constants for $H^o(T)/RT$ and $S^o(T)/R$ . The NASA Glenn computer program PAC (Properties and Coefficients) was used to calculate thermodynamic functions and to generate the least-squares coefficients. PAC input was taken from a variety of sources. A complete listing of the database is given along with a summary of thermodynamic properties at 0 and 298.15 K.				
14. SUBJECT TERMS  Heats of formation; CEA; McBride; Gordon; Thermodynamics; Thermodynamic properties; NASA; NASA Lewis; Specific heat; NASA Glenn; Enthalpy; Entropy; Heat capacity			15. NUMBER OF PAGES 291	
			16. PRICE CODE	
17. SECURITY CLASSIFICATION OF REPORT  Unclassified	18. SECURITY CLASSIFICATION OF THIS PAGE  Unclassified	19. SECURITY CLASSIFICATION OF ABSTRACT  Unclassified	20. LIMITATION OF ABSTRACT	





