THE-036-1
CHEMKIN Collection Release 3.6
September 2000

THE CHEMKIN THERMODYNAMIC DATABASE

Reaction Design

Licensing:

For licensing information, please contact Reaction Design.
(858) 550-1920 (USA) or CHEMKIN@ReactionDesign.com

Technical Support:

Reaction Design provides an allotment of technical support to its Licensees free of charge. To request technical support, please include your license number along with input or output files, and any error messages pertaining to your question or problem. Requests may be directed in the following manner: E-Mail: Support@ReactionDesign.com, Fax: (858) 550-1925, Phone: (858) 550-1920.
Technical support may also be purchased. Please contact Reaction Design for the technical support hourly rates at Support@ReactionDesign.com or (858) 550-1920 (USA).

Copyright:

Copyright© 2000 Reaction Design. All rights reserved. No part of this book may be reproduced in any form or by any means without express written permission from Reaction Design.

Trademark:

AURORA, CHEMKIN, The CHEMKIN Collection, CONP, CRESLAF, EQUIL, Equilib, OPPDIF, PLUG, PREMIX, Reaction Design, SENKIN, SHOCK, SPIN, SURFACE CHEMKIN, SURFTHERM, TRANSPORT, TWOPNT are all trademarks of Reaction Design or Sandia National Laboratories.

Limitation of Warranty:

The software is provided "as is" by Reaction Design, without warranty of any kind including without limitation, any warranty against infringement of third party property rights, fitness or merchantability, or fitness for a particular purpose, even if Reaction Design has been informed of such purpose. Furthermore, Reaction Design does not warrant, guarantee, or make any representations regarding the use or the results of the use, of the software or documentation in terms of correctness, accuracy, reliability or otherwise. No agent of Reaction Design is authorized to alter or exceed the warranty obligations of Reaction Design as set forth herein.

Any liability of Reaction Design, its officers, agents or employees with respect to the software or the performance thereof under any warranty, contract, negligence, strict liability, vicarious liability or other theory will be limited exclusively to product replacement or, if replacement is inadequate as a remedy or in Reaction Design's opinion impractical, to a credit of amounts paid to Reaction Design for the license of the software.

Literature Citation for the CHEMKIN THERMODYNAMIC DATABASE:

The CHEMKIN THERMODYNAMIC DATABASE is part of the *CHEMKIN Collection*.

R. J. Kee, F. M. Rupley, J. A. Miller, M. E. Coltrin, J. F. Grcar, E. Meeks, H. K. Moffat, A. E. Lutz, G. Dixon-Lewis, M. D. Smooke, J. Warnatz, G. H. Evans, R. S. Larson, R. E. Mitchell, L. R. Petzold, W. C. Reynolds, M. Caracotsios, W. E. Stewart, P. Glarborg, C. Wang, and O. Adigun, *CHEMKIN Collection*, Release 3.6, Reaction Design, Inc., San Diego, CA (2000).

Acknowledgements:

This document is based on the Sandia National Laboratories Report SAND87-8215B, authored by R. J. Kee, F. M. Rupley, and J. A. Miller.[1]

Reaction Design cautions that some of the material in this manual may be out of date. Updates will be available periodically on Reaction Design's web site. In addition, on-line help is available on the program CD. Sample problem files can also be found on the CD and on our web site at www.ReactionDesign.com.

THE CHEMKIN THERMODYNAMIC DATABASE

ABSTRACT

The Chemkin Thermodynamic database contains polynomial fits to specific heats, standard state enthalpies, and standard state entropies. These fits are used by the Chemkin Collection, a general-purpose chemical kinetics software package. The fourteen coefficients for each species are in the same form as used in the NASA Complex Chemical Equilibrium Program.2 This manual provides details on the compilation of the data that is currently part of the Chemkin Collection, including graphical representations of the fits to experimental (or calculated) data points. Also included is a description of a fitting utility program called Fitdat. Fitdat can be used to generate the Chemkin–compatible fitting coefficients from tables of specific heats, entropies, and enthalpies vs. temperature, as well as from vibrational-frequency values.

CONTENTS

LIST OF FIGURES

LIST OF TABLES

1. Introduction

This manual documents the thermodynamic property database that is an integral part of the CHEMKIN Collection, a chemical kinetics software package. Further documentation on CHEMKIN and CHEMKIN Applications are provided in the user's manuals for those programs. Briefly, CHEMKIN is composed of four important pieces: the Interpreter, the Thermodynamic Database, the Linking file, and the Gas-Phase Subroutine library. The Interpreter is a program that first reads the user's symbolic description of the reaction mechanism. It then extracts thermodynamic information for the species involved from the Thermodynamic Database. The user may add to or modify the information in the database by input to the Interpreter. In addition to printed output, the Interpreter writes a Linking File, which contains all the pertinent information on the elements, species, and reactions in the mechanism.

Once the CHEMKIN Interpreter has been executed and the Linking file created, the user is ready to use a CHEMKIN Application, which accesses the Gas-Phase Subroutine Library. Applications call the CHEMKIN subroutines as needed to return information on the elements, species, reactions, equations of state, thermodynamic properties, chemical production rates, sensitivity parameters, derivatives of chemical production rates, and derivatives of thermodynamic properties. Generally, the input to these subroutines is the state of the gas – pressure or density, temperature, and the species composition.

Originally, the CHEMKIN software package and its applications were developed for use in combustion simulations. The combustion studies concentrated on small molecule hydrocarbon systems, especially those involving the nitrogen chemistry responsible for producing nitrogen-oxygen based pollutants. The most comprehensive parts of the database, then, are the thermodynamic properties for species important in such combustion systems. Focused studies of the chemical vapor deposition of silicon from silane at Sandia National Laboratories also led to enhancements of the database, with inclusion of several silicon-hydrogen compounds.

This manual first explains how the polynomial fits to the property data are generated. Then in three appendices we present the data itself in several formats. Appendix A lists the standard state heats of formation and entropies at 298 K for each of the species in the database. Appendix B is a listing of the database in the form that CHEMKIN expects to find it. Finally, Appendix C presents a graphical account of the properties as a function of temperature. Where available, the actual data from which the fits were determined are also plotted to indicate the accuracy of the fit. Also in Appendix C is a reference to the source of the data used in the fitting process.

2. The Data Sources

The data originates from three major sources. First is the set of JANAF[3] tables. Generally speaking, if available, JANAF is the preferred source of our data. The properties of many hydrocarbon species not included in the JANAF compilations come from the compilation of Burcat[4]. In this case, the data provided by Burcat is already fit in the form required for our database. The third source of data is quantum chemistry computations.

Calculation of thermochemical data using high-quality *ab initio* electronic structure calculations has been a long-standing goal. However, the availability of supercomputers and new theoretical techniques now allow the calculation of thermochemical properties with chemical accuracy, i.e., ΔH_f to within ± 3 kcal/mole. A technique that has been applied to over 900 combustion-related chemical species and to our study of silicon-containing species is denoted the BAC-MP4 method[5-9]. It combines electronic structure calculations using fourth-order Møller-Plesset perturbation theory[10-12] (MP4) with empirically derived bond additivity correction (BAC) factors to account for systematic error in the *ab initio* calculations due to truncated wave functions and incomplete basis sets.

3. The Fitting Procedure

The data format used is a minor modification of that used by Gordon and McBride[13] for the thermodynamic database in the NASA Chemical Equilibrium program. The thermodynamic data are stored as polynomial fits to specific heat c_P/R, enthalpy H^0/RT, and entropy S^0/R. There are seven coefficients for each of two temperature-ranges.

$$\frac{c_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \tag{1}$$

$$\frac{H^0}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \tag{2}$$

$$\frac{S^0}{R} = a_1 1nT + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \tag{3}$$

Thus for each species there are 14 coefficients in all. In addition to the polynomial coefficients for each species, the Thermodynamic Database provides the species name, its elemental makeup, and the temperature ranges over which the fits are valid.

The essential input to the fitting procedure is a table of specific heat, enthalpy, and entropy as a function of temperature. In addition since the fits span two temperature ranges, the temperature ranges have to be specified. Generally speaking, the common temperature connecting the two ranges is 1000 K, but it may be different in some cases.

The constrained linear least squares fitting procedure[14, 15] is a three stage process. The first step is to determine simultaneously a_1 through a_5 for both temperature ranges by fitting the specific heats to Eq. (1). The fitting procedure is constrained such that at the common temperature both the specific heat and its first derivative are equal. The second step is to determine a_6 for both temperature ranges by fitting the enthalpy data. In this state, a_1 – a_5 are held fixed, and as in the c_p fitting, equality constraints on the fit and its first derivative are imposed at the common temperature. Finally, the a_7 coefficients are determined by fitting the entropy data. Again, the $a_1 - a_5$ coefficients are held fixed and the equality constraints are imposed at the common temperature. We note that this fitting procedure is slightly different from the procedure followed by McBride and Gordon,[2] who fit all coefficients simultaneously.

4. The FITDAT Fitting Program

FITDAT is a program that performs a least-squares fitting procedure for thermodynamic data. The program accepts a molecule description in the form of character-string keywords, followed by thermodynamic data values. The thermodynamic data input takes the form of a table of specific heat, enthalpy, and entropy values as functions of temperature. Alternately, the FITDAT program accepts as input molecular vibrational frequencies, which are then used to extrapolate the thermodynamic functions. The default output is the set of polynomial fitting coefficients for each of two temperature-ranges, as required by the CHEMKIN Interpreter. An optional output format is also available for using more than two temperature-ranges.

The FITDAT program is written in Fortran77, and requires linking with the public math subroutines provided by Reaction Design, or available to the public from other sources. As distributed, FITDAT is dimensioned to accept up to 100 function values. Source code for the fitting routine is provided as part of the standard CHEMKIN distribution.

Although error diagnostics are provided by the program, we strongly advise verifying the quality of the polynomial fits by exporting the results to a graphical post-processor.

4.1 Example FITDAT Input

```
! Sample input for fitting data with equality constraints
! * means the keyword and data is optional, else the keyword is required
! exclamation (!) may be used for comments
!
!DIAG 1          ! * print relative error diagnostics (default=NO)
DIAG 2           ! * print relative errors, plus table of Cp,H,S data vs. fit
values
!DATE 032800     ! * fill date field in output
SPEC OH          !   species name
ELEM O 1         !   elemental composition
ELEM H 1
TEMP 1000        ! * equality constraint (default=none)
TMIN 300         ! * start temperature for fit (default=300)
                 !   if TMIN > first data point, truncate input data
!TMAX 6000       ! * end temperature for fit (default=last data point given),
                 !   if TMAX < last data point, truncate input data
                 !   if TMAX > last data point, extrapolate TMAX data
H298 9.32        !   formation enthalpy @298K, Kcal/mole
! S298 43.88     ! * formation entropy @298K, cal/mole
LINR N           ! * linearity of molecule (Y/N)
DATA             !   start of table, 4 columns to follow,
                 !   T(K), Cp(cal/mole-K), S(cal/mole K), H(Kcal/mole)
0300.00  007.165  043.926  000.013
0400.00  007.087  045.974  000.725
0500.00  007.056  047.552  001.432
   :        :        :        :
   :        :        :        :
4900.00  009.232  065.778  038.571
5000.00  009.249  065.965  039.495
END              ! END required to start processing data
!
! Sample input for fitting with vibrational frequencies input
!
DIAG 2           !* 1, print max relative error;
                 !  2, also print data
                 ! (default=0)
SPEC SIH2        !  species symbol
PHAS G           !* G,L,S (default='G')
LINR N           !* linearity of molecule (default 'Y' if 1 VIBE,else 'N')
TEMP 1000        !* equality constraint (default is one range, no equality
                 !    constraint)
TMAX 5000        !* max temperature for fitting (default=6000)
TMIN 300         !* min temperature
ELEM SI 1        !  elemental composition
ELEM H2 1
VIBE  999.83     !  vibrational frequency, cm-1
VIBE 2011.69
VIBE 2001.72
H298 58.0        !  formation enthalpy @298K, Kcal/mole
S298 49.4        !  formation entropy @298K, cal/mole
END
```

4.2 Example FITDAT Output

The FITDAT program will produce both an output diagnostics file (which may also be written to standard output) and a text file containing the fitting coefficients. The polynomial fitting coefficients will be output to a file named "fitdat.txt". The following are examples of output generated with the input in Section 4.1.

4.2.1 POLYNOMIAL COEFFICIENTS

```
OH                      0O   1H   1    0    0G   300.000  5000.000 1000.00    0 1
 0.28952326E+01 0.10120984E-02-0.23692351E-06 0.26039484E-10-0.10187232E-14    2
 0.38761752E+04 0.55131778E+01 0.34533338E+01 0.15747093E-02-0.52733631E-05    3
 0.61786813E-08-0.22379330E-11 0.36248042E+04 0.21219087E+01                   4
SIH2                    0SI  1H   2    0    0G   300.000  5000.000 1000.00    0 1
 0.34567856E+01 0.37123408E-02-0.15670881E-05 0.29779442E-09-0.21039015E-13    2
 0.27914508E+05 0.39288294E+01 0.46212792E+01-0.58395360E-02 0.20101580E-04    3
-0.19041887E-07 0.60373568E-11 0.27926304E+05-0.46570373E+00                   4
```

4.2.2 POLYNOMIAL COEFFICIENTS FOR MORE THAN TWO TEMPERATURE-RANGES

The following results would be obtained for the same input data as above, but using two equality constraints, resulting in three temperature ranges. For this output, both "TEMP 1000" and "TEMP 2500" were included in the keyword input:

```
OH                      0O   1H   1    0    0G   300.000  5000.000           0 1
TEMP   300.000  1000.000  2500.000  5000.000
 0.30563941E+01 0.89059362E-03-0.20849917E-06 0.24115927E-10-0.10516720E-14
 0.37260112E+04 0.44780081E+01
 0.34298433E+01-0.25250392E-03 0.80470663E-06-0.33336490E-09 0.43425671E-13
 0.37097800E+04 0.26751302E+01
 0.37695923E+01-0.59256858E-03-0.21359336E-06 0.13644331E-08-0.63575666E-12
 0.35908836E+04 0.78130486E+00
```

4.2.3 DIAGNOSTICS

```
Species OH Diagnostics:
     T      Cp data/R   Cp/R fit       relative error
   300.00   0.361E+01   0.360E+01         0.161E-02
   400.00   0.357E+01   0.358E+01         0.315E-02
   500.00   0.355E+01   0.355E+01         0.113E-02
     :        :           :               :
     :        :           :               :
  4900.00   0.465E+01   0.464E+01         0.772E-03
  5000.00   0.465E+01   0.465E+01         0.752E-03
 The maximum relative CP error was  0.400E-02 at T= 700.000
```

5. Database Management

The CHEMKIN database requires four fixed format records to represent the properties for each species. This is consistent with other databases, such as the used in the NASA Chemical Equilibrium Code.[13] However, while this format is complete enough to describe the properties, it contains only the bare minimum data needed. At present the complete database is maintained by using a relational database software system.

The database contains the following fields:

1. Identification – chemical symbol, species name, elemental composition, and phase;
2. Fit coefficients for the thermodynamic properties, and the temperature ranges for which they apply.
3. Data used to generate the fit, if available. These fields contain $H^0(298)$, $S^0(298)$, and tables of $c_p(T)$, $S^0(T)$, $H^0(T)$ as functions of temperature.
4. References – source of data, date, any relevant comments.

Using a relational database manager provides considerably more flexibility in managing the data than the original CHEMKIN database. Various types of reports can be produced from database manager programs. The appendices in this manual represent three examples of such reports.

6. References

1. R. J. Kee, F. M. Rupley, and J. A. Miller, "The Chemkin Thermodynamic Data Base" Sandia National Laboratories Report SAND87-8215B (1990).
2. B. J. McBride and S. Gordon, "FORTRAN IV Program for Calculation of Thermodynamic Data" NASA Report NASA TN-4097 (1967).
3. JANAF, "Thermochemical Tables, National Standards Reference Data Series" Report NSRDS-NBS 37: also Dow Chemical Company, distributed by Clearinghouse for Federal Scientific and Technical Information, PB168370 (1965) and subsequent updates (1965).
4. A. Burcat, in Combustion Chemistry, edited by W. C. Gardiner (Springer Verlag, New York, 1984), p. 455.
5. C. F. Melius and J. S. Binkley, in Proceedings of the Fall Meeting of the Western States Section of the Combustion Institute, University of California, Los Angeles, CA (1983).
6. C. F. Melius and J. S. Binkley, in Proceedings of the 20th Symposium (International) on Combustion, Combustion Institute, Pittsburgh, p. 575 (1984).
7. C. F. Melius and J. S. Binkley, ACS Symposium Series 249: 103 (1984).
8. P. Ho, M. E. Coltrin, J. S. Binkley, and C. F. Melius, J. Physical Chemistry 89: 4647 (1985).
9. P. Ho, M. E. Coltrin, J. S. Binkley, and C. F. Melius, J. Physical Chemistry 90: 3399 (1986).
10. J. A. Pople, J. S. Binkley, and R. Seeger, International J. Quantitative Chemistry S10: 1 (1976).
11. R. Krishnan and J. A. Pople, International J. Quantitative Chemistry 14: 91 (1978).
12. R. Krishnan, M. J. Frisch, and J. A. Pople, J. Chemical Physics 72: 4244 (1980).
13. S. Gordon and B. J. McBride, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks and Chapman-Jouguet Detonations" NASA Report SP-273 (1971).
14. R. J. Hanson and K. H. Haskell, "Algorithms for Linear Least Squares Problems with Equality and Non-negativity Constraints" Sandia National Laboratories Report SAND77-0552 (1978).
15. R. J. Hanson and K. H. Haskell, "Selected Algorithms for Linearly Constrained Least Squares Problems - A Users Guide" Sandia National Laboratories Report SAND78-1290 (1979).

Appendix A. Standard State Enthalpies and Entropies at 298 K

This Appendix contains the standard state enthalpies and entropies for 778 species that are in the CHEMKIN Thermodynamic Database "therm.dat" (See Appendix B, Tables B.1 and B.2 for the data and formats). The values in the table were determined by evaluating the polynomial expressions (1-2) at the standard temperature of 298 K. (Note the measured or derived data for $H^0(298)$ and $S^0(298)$ that were used in generating the coefficients in the first place are maintained in a separate file)

$$H^0(298) = RT\left[a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T}\right] \tag{A.1}$$

$$S^0(298) = R\left[a_1 1nT + a_2 T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7\right] \tag{A.2}$$

The units for enthalpies are Kcal/mole and for entropies cal/mole-K. The database corresponds to the "therm.dat" distributed with CHEMKIN Collection Release 3.6.

Table A.1 Standard State Enthalpies and Entropies at 298 K.

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
(CH2O)3	-110.70	-110.71	69.42	69.38
(CH3)2SICH2	12.30	12.37	80.37	82.41
AL	78.80	78.80	39.30	39.30
AL2H6	21.35	21.35	62.75	62.75
AL2ME6	-61.20	-61.20	131.05	131.06
ALAS	107.33	107.32	60.65	60.65
ALH	62.00	62.00	44.88	44.87
ALH2	41.95	41.95	54.40	54.40
ALH3	18.83	18.83	52.30	52.30
ALME	19.75	19.75	60.68	60.68
ALME2	12.75	12.75	77.40	77.40
ALME3	-20.30	-20.30	83.68	83.68
AR	0.00	0.00	36.98	36.98
AR+	364.91	364.91	39.75	39.74
AS	75.48	75.48	43.53	43.52
AS2	47.08	47.08	59.83	59.83
AS3	65.35	65.35	77.53	77.53
AS4	37.13	37.13	78.45	78.45
ASALME	70.00	70.00	81.60	81.60
ASALME2	63.25	63.25	91.00	91.00
ASGAET	82.75	82.75	95.20	95.20
ASGAET2	69.55	69.55	109.83	109.83
ASGAME	83.50	83.50	85.75	85.75
ASGAME2	81.25	81.25	91.00	91.00
ASGAMEH	93.75	93.75	84.73	84.73
ASH	61.75	61.75	50.20	50.20
ASH2	42.25	42.25	46.45	46.45
ASH3	16.63	16.63	55.65	55.65
ASME	59.20	59.20	63.80	63.80
ASME2	34.20	34.20	79.50	79.50
ASME3	2.93	2.93	85.78	85.78
B	133.80	133.80	36.65	36.64
B(S)	0.00	0.00	1.41	1.41
BCL	33.80	33.80	50.94	50.94
BCL2	-19.00	-19.00	65.14	65.15

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
BCL3	-96.31	-96.31	69.33	69.33
BE	78.25	78.25	32.54	32.54
BE(S)	0.00	0.00	2.28	2.28
BE2SIO4(S)	-506.03	-506.03	15.34	15.33
BE3B2O6(S)	-741.96	-741.96	24.00	23.97
BE3N2(A)	-140.60	-140.60	8.16	8.15
BE3N2(L)	-116.40	-116.41	9.43	9.41
BEAL2O4(S)	-549.90	-549.90	15.84	15.84
BEB2O4	-323.00	-323.00	78.08	78.08
BEBO2	-115.20	-115.20	63.40	63.41
BEBR	28.71	28.71	54.59	54.59
BEBR2	-54.80	-54.80	65.44	65.44
BEBR2(S)	-85.00	-85.00	24.00	23.99
BECL	14.50	14.50	51.98	51.98
BECL2	-86.10	-86.10	60.26	60.26
BECL2(A)	-117.34	-117.34	19.76	19.75
BECL2(B)	-118.60	-118.60	18.12	18.11
BECLF	-137.00	-137.00	58.89	58.89
BEF	-40.60	-40.60	49.15	49.14
BEF2	-190.25	-190.25	54.36	54.36
BEF2(L)	-244.27	-244.28	14.32	14.32
BEH	76.77	76.77	42.24	42.23
BEH+	276.40	276.40	40.76	40.75
BEH2	30.00	30.00	41.35	41.33
BEH2O2	-161.70	-161.70	55.89	55.91
BEH2O2(A)	-215.80	-215.81	12.80	12.78
BEH2O2(B)	-216.50	-216.51	12.00	11.98
BEI	40.63	40.63	56.69	56.69
BEI2	-15.30	-15.30	69.65	69.65
BEI2(S)	-45.10	-45.11	28.80	28.78
BEN	101.98	101.98	49.87	49.87
BEO(A)	-145.40	-145.39	3.29	3.31
BEO(B)	-143.80	-143.79	3.97	3.99
BEOH	-27.40	-27.40	50.07	50.07
BES(S)	-56.00	-56.00	8.85	8.84
BESO4(A)	-287.00	-287.01	18.64	18.60

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
BESO4(B)	-286.73	-286.75	18.94	18.91
BESO4(GAM)	-282.06	-282.07	24.09	24.06
BN	-59.97	-59.97	3.54	3.53
C	171.29	171.29	37.76	37.76
C(S)	0.00	0.00	1.37	1.37
C+	432.47	432.02	36.94	36.93
C-	140.61	140.61	36.16	36.16
C2	200.22	200.23	47.63	47.63
C2-	106.00	106.00	46.96	46.96
C2CL3	54.37	54.36	79.93	79.89
C2CL5	7.38	7.39	94.52	94.75
C2CL6	-32.43	-32.44	93.15	93.04
C2F6	-321.20	-321.20	79.37	79.38
C2H	135.00	135.00	51.10	49.55
C2H2	54.19	54.19	48.00	48.01
C2H3	0.00	68.41	0.00	55.32
C2H4	12.54	12.54	52.40	52.37
C2H5	0.00	28.01	0.00	60.13
C2H6	0.00	-20.04	0.00	54.72
C2HCL	51.10	51.10	57.81	57.82
C2HCL5	-35.19	-35.19	91.61	91.51
C2N	133.00	133.00	55.16	55.16
C2N2	73.87	73.87	57.71	57.72
C2O	68.50	68.50	55.68	55.67
C3	196.00	196.00	56.68	56.66
C3H2	129.39	129.60	62.01	64.81
C3H2(S)	141.43	141.43	59.74	59.75
C3H4	47.67	47.63	57.99	57.94
C3H4C	67.99	68.00	57.94	57.95
C3H4P	45.77	45.77	58.89	58.89
C3H6	0.00	4.89	0.00	61.51
C3H8	0.00	-24.82	0.00	64.56
C3O2	-22.38	-22.38	65.96	65.96
C4	232.00	232.00	54.54	54.55
C4H	0.00	155.08	0.00	60.89
C4H10	-32.02	-31.84	70.94	71.79

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
C4H2	0.00	111.70	0.00	59.77
C4H6	0.00	34.96	0.00	68.16
C4H8	0.00	-0.13	0.00	73.55
C5	234.00	234.01	57.81	57.82
C5H	0.00	185.99	0.00	62.20
C5H12	0.00	-34.98	0.00	83.48
C5H2	0.00	165.23	0.00	63.69
C5H5	63.83	63.84	68.10	68.13
C5H6	0.00	31.99	0.00	64.45
C6H	0.00	213.15	0.00	74.10
C6H10	0.00	-1.00	0.00	74.75
C6H14	0.00	-39.91	0.00	92.87
C6H2	0.00	169.66	0.00	70.92
C6H3	0.00	158.45	0.00	76.30
C6H4	99.66	99.67	68.25	68.26
C6H5	79.42	79.43	69.81	69.82
C6H5(L)	140.58	140.58	83.39	84.26
C6H5O	10.34	10.35	74.86	74.87
C6H5OH	-25.13	-25.01	76.96	76.93
C6H6	0.00	19.81	0.00	64.35
C6H7	47.94	47.96	73.07	73.07
C8H	0.00	288.86	0.00	78.39
C8H2	0.00	226.15	0.00	75.94
CA	42.85	42.85	36.99	36.98
CA(A)	0.00	0.00	9.93	9.93
CA(B)	0.12	0.12	10.15	10.15
CA(L)	2.61	2.60	12.11	12.10
CA+	185.30	185.30	38.37	38.37
CA2	82.66	82.66	61.29	61.29
CABR	-11.81	-11.81	60.42	60.41
CABR2	-92.00	-92.00	75.20	75.20
CABR2(S)	-163.30	-163.30	31.00	30.99
CACL	-25.00	-25.00	57.71	57.71
CACL2	-112.70	-112.70	69.35	69.35
CACL2(S)	-190.20	-190.20	25.00	24.99
CAF	-65.00	-65.00	54.86	54.86

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
CAF2	-187.50	-187.50	65.41	65.42
CAH2O2	-145.98	-145.97	68.23	68.25
CAH2O2(S)	-235.68	-235.68	19.93	19.93
CAI	-1.21	-1.21	62.43	62.42
CAI2	-61.70	-61.70	78.26	78.26
CAO	10.50	10.50	52.49	52.52
CAO(S)	-151.79	-151.79	9.13	9.15
CAOH	-46.34	-46.34	56.25	56.26
CAOH+	88.21	88.21	54.92	54.93
CAS	29.54	29.52	55.56	55.55
CCL	106.10	106.10	52.46	52.45
CCL2	53.02	53.02	63.29	63.28
CCL2CCLO	-24.27	-24.27	85.06	84.97
CCL2CCLOH	-44.66	-44.69	83.09	82.88
CCL2CH	62.30	62.29	71.95	71.93
CCL2HOO	-1.37	-1.33	78.30	79.17
CCL2OHCH2	-22.77	-22.60	79.91	80.63
CCL2OHCHCL	-31.69	-31.54	87.57	89.10
CCL3	16.58	16.58	72.20	72.20
CCL3CCLH2	-35.29	-35.28	85.57	85.59
CCL3CCLO	-56.49	-56.47	89.99	90.43
CCL3CH2	18.79	18.89	81.61	82.80
CCL3CHCL	11.06	11.09	88.40	89.03
CCL3CHO	-45.51	-45.47	83.71	85.04
CCL3OO	-0.74	-0.71	83.14	83.46
CCL4	-20.22	-20.22	78.91	78.91
CCLH2OO	1.22	1.27	71.06	71.68
CH	142.00	142.00	43.72	43.71
CH+	388.80	388.80	41.00	41.00
CH2	92.48	92.48	46.72	46.71
CH2(S)	101.50	101.50	45.10	45.10
CH2CCL	61.43	61.39	64.24	64.15
CH2CCL2	0.75	0.71	68.84	68.76
CH2CCLOH	-37.01	-36.94	69.00	69.35
CH2CHCCH	69.14	69.14	66.49	67.33
CH2CHCCH2	74.11	74.14	74.70	75.31

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
CH2CHCH2	38.70	38.64	64.39	64.73
CH2CHCHCH	86.13	86.09	72.75	73.06
CH2CHCHCH2	28.33	28.29	69.74	70.44
CH2CHCL	4.69	4.67	63.03	62.98
CH2CL	27.08	27.07	59.28	59.28
CH2CL2	-22.83	-22.83	64.57	64.57
CH2CLCCL2	6.02	6.05	82.70	83.32
CH2CLCCLO	-58.33	-58.30	77.51	78.10
CH2CLCH2	23.00	23.10	68.36	69.46
CH2CLCH2CL	-32.35	-32.33	72.20	72.45
CH2CLCHCL	13.10	13.14	75.92	76.80
CH2CLCHCL2	-35.23	-35.22	80.05	80.12
CH2CLCHO	-41.67	-41.66	72.11	74.04
CH2CO	0.00	-12.40	0.00	57.78
CH2F2	-107.71	-107.71	58.94	58.91
CH2HCO	0.00	6.00	0.00	63.99
CH2O	-27.70	-27.70	52.26	52.24
CH2OH	-4.21	-4.10	58.93	58.87
CH2OHCCL2	-23.26	-23.21	82.18	82.65
CH2OHCHCL	-16.90	-16.79	74.35	74.94
CH2SICL	45.68	45.67	69.39	69.33
CH2SICL3	-87.71	-87.71	90.16	91.94
CH2SIH2CL	-0.90	-0.87	74.23	75.92
CH2SIHCL2	-44.67	-44.67	83.30	85.08
CH3	34.82	34.82	46.38	46.37
CH3C(O)CL	-56.93	-56.86	70.60	71.87
CH3CC	123.81	123.82	60.28	60.27
CH3CCCH2	74.33	74.34	78.57	80.35
CH3CCCH3	40.92	40.94	71.58	73.36
CH3CCH2	61.04	61.09	69.12	69.24
CH3CCL	61.68	61.73	66.18	67.81
CH3CCL2	10.33	10.42	75.42	76.27
CH3CCL3	-33.55	-33.51	76.48	76.61
CH3CCLO	-56.93	-56.86	70.60	71.87
CH3CH2CCH	44.66	44.75	71.46	71.43
CH3CH2CH2CH3	-30.64	-30.50	72.68	73.31

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
CH3CH2CL	-27.17	-27.10	66.00	66.33
CH3CH2O	-0.51	-0.44	65.48	65.81
CH3CHCH	64.70	64.75	68.49	68.74
CH3CHCL	18.22	18.30	68.46	69.48
CH3CHCL2	-32.08	-32.02	72.79	73.04
CH3CHOH	-14.34	-14.17	66.73	67.77
CH3CL	-20.00	-20.00	55.99	55.97
CH3CO	0.00	-5.40	0.00	63.73
CH3F	-56.00	-56.00	53.25	53.22
CH3HCO	0.00	-39.51	0.00	63.04
CH3NO	18.88	18.95	62.33	63.46
CH3NO2	-16.83	-16.84	70.26	72.03
CH3O	0.00	3.89	0.00	54.60
CH3OCH3	-43.80	-43.72	63.74	64.35
CH3OCL	-14.06	-13.98	64.97	65.42
CH3OH	0.00	-48.06	0.00	57.27
CH3ONO	-15.30	-15.25	66.63	66.87
CH3ONO2	-26.12	-26.06	71.34	71.63
CH3SICL	-2.47	-2.44	70.99	72.63
CH3SIH2SIH	-10.12	-9.96	88.03	91.66
CH3SIH2SIH2CH3	-10.92	-10.79	88.03	90.60
CH3SIHCL2	-93.81	-93.74	79.61	80.53
CH4	-17.90	-17.90	44.49	44.46
CHCL	80.00	80.00	56.12	56.11
CHCL2	19.51	19.51	65.08	65.08
CHCL2CCL2	8.53	8.53	90.99	92.74
CHCL2CCLO	-57.87	-57.85	84.59	85.22
CHCL2CH2	20.23	20.24	78.03	79.99
CHCL2CHCL	10.32	10.35	82.79	83.54
CHCL2CHCL2	-36.03	-36.02	85.18	85.39
CHCL3	-23.25	-23.25	70.64	70.64
CHCLCCL	55.99	55.98	72.48	72.40
CHCLCCLOH	-43.59	-43.51	76.26	76.42
CHCLCH	64.77	64.81	64.47	64.48
CHCLCHCL	-1.15	-1.15	69.24	69.19
CHCLCHOH	-38.64	-38.56	68.93	69.13

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
CHCLOH	-16.71	-16.65	65.30	65.41
CHCLOHCH2	-15.20	-15.08	74.53	76.30
CHCLOHCHCL	-24.95	-24.85	82.31	83.81
CHF	30.00	30.00	53.36	53.35
CHF3	-166.60	-166.60	62.03	62.02
CHOHCLCCL2	-31.95	-31.84	88.72	90.27
CHSICL	89.13	89.13	70.30	70.30
CHSICL2	29.60	29.61	81.07	82.86
CHSICL3	-35.28	-35.27	88.41	90.19
CHSIH2CL	50.52	50.55	73.11	74.85
CHSIHCL	67.86	67.93	70.62	72.26
CHSIHCL2	7.19	7.22	80.87	82.62
CL	28.99	28.99	39.45	39.45
CL(CH3)SICH2	-13.11	-13.08	78.44	79.58
CL2	0.00	0.00	53.29	53.29
CL2CCCL2	-5.66	-5.67	81.51	81.41
CL2CCHCL	-3.95	-3.96	77.64	77.54
CL2CCHO	-12.45	-12.46	77.67	77.57
CL2CHOH	-66.56	-66.41	71.53	72.50
CL2CO	-52.70	-52.70	67.64	67.64
CL2COH	-22.80	-22.68	73.07	73.68
CL2HCO	-4.12	-4.12	71.65	71.64
CL2SI(CH3)2	-113.74	-113.59	88.72	90.45
CL2SI(CH3)CH2	-64.26	-64.18	92.21	94.86
CL2SICH2	-34.22	-34.25	75.18	75.10
CL2SICH3	-52.78	-52.71	80.76	81.74
CL2SISI	32.71	32.71	79.88	79.88
CL2SISICL	-24.42	-24.41	92.40	92.46
CL2SISICL2	-95.69	-95.69	102.08	102.02
CL3CCO	1500.00	1500.02	-5.27	87.34
CL3CO	-4.37	-4.37	78.35	78.35
CL3COH	-66.33	-66.23	77.64	79.21
CL3SICH3	-137.81	-137.74	84.47	85.28
CL3SISI	-26.17	-26.17	89.43	89.43
CL3SISICL	-99.56	-99.55	101.49	103.27
CLCCCL	56.20	56.20	64.28	64.28

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
CLCCO	42.24	42.25	68.92	68.87
CLCH2OH	-55.49	-55.49	69.49	71.45
CLCO	-6.48	-6.48	64.39	64.39
CLCOH	1.17	1.13	62.43	62.37
CLH2CO	-2.35	-2.35	64.42	64.41
CLHCO	-44.30	-44.30	61.80	61.79
CLO	29.20	29.19	53.00	52.99
CLOCL	19.71	19.71	63.65	63.65
CLOO	33.60	33.60	63.54	63.53
CLSI(CH3)2	-26.19	-26.06	82.72	84.80
CLSI(CH3)2CH2	-37.20	-37.04	92.86	96.44
CLSI(CH3)3	-86.29	-86.08	90.84	93.65
CLSICH3	-2.86	-2.82	70.99	72.64
CLSISI	99.11	99.11	71.44	71.44
CLSISICL	33.48	33.48	81.76	81.88
CN	104.00	104.00	48.41	48.40
CN+	430.87	430.87	50.99	50.98
CN-	14.50	14.50	46.81	46.81
CN2	113.00	113.00	54.04	54.03
CNN	139.70	139.70	55.35	55.35
CNO	97.64	97.64	55.57	55.57
CO	-26.42	-26.42	47.21	47.21
CO2	-94.05	-94.05	51.07	51.07
CO2-	-105.50	-105.50	57.49	57.48
COS	-33.08	-33.08	55.32	55.33
CS	67.00	67.00	50.30	50.29
CS2	27.95	27.95	56.85	56.85
CSICL	146.05	146.06	68.07	68.07
CSICL2	89.11	89.11	76.71	76.71
CSICL3	9.05	9.05	86.79	86.79
CSIH2CL	105.85	105.85	69.88	69.88
CSIHCL	119.47	119.47	67.68	67.68
CSIHCL2	63.16	63.16	77.47	77.47
D	52.99	52.99	29.46	29.45
D2	0.00	0.00	34.62	34.62
DH	0.08	0.08	34.34	34.34

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
DIOXANE	-75.11	-75.12	71.76	71.72
E	0.00	0.00	0.00	4.98
F	18.90	18.90	36.15	36.14
F-	-61.08	-61.08	34.77	34.76
F2	-0.09	-0.09	48.14	48.14
F2N2(C)	16.40	16.40	62.07	62.08
F2O2	14.00	13.99	64.42	64.33
F2SINH	-146.95	-146.93	70.92	70.92
F3SIN	-200.02	-200.02	73.86	73.87
FNNF	17.88	17.88	63.07	63.47
FNO3	2.50	2.50	69.99	69.99
FO	26.00	26.00	51.77	51.76
FO2	3.00	3.00	61.90	61.90
FONO(C)	10.18	10.16	64.43	64.34
FONO(T)	14.13	14.12	64.88	64.79
FSIN	54.37	54.37	63.67	63.67
GA	68.53	68.52	43.83	43.82
GA2H6	31.50	31.50	69.05	69.05
GAAS	88.40	88.40	63.23	63.23
"GAAS(3,C)"	245.75	245.75	100.00	100.00
"GAAS(3,L)"	256.25	256.25	127.75	127.75
"GAAS(5,C)"	357.75	357.75	130.50	130.50
"GAAS(5,L)"	420.00	420.00	193.50	193.50
GAET	17.75	17.75	81.60	81.60
GAET2	4.50	4.50	100.43	100.43
GAET3	-17.05	-17.05	112.98	112.98
GAH	54.80	54.80	49.18	49.17
GAH2	41.00	41.00	56.00	56.00
GAH3	27.00	27.00	54.50	54.50
GAME	18.53	18.53	63.80	63.80
GAME2	16.42	16.43	80.55	80.55
GAME3	-10.88	-10.87	87.88	87.88
H	52.10	52.09	27.39	27.39
H(CH3)SICH2	26.36	26.39	70.27	71.37
H+	367.17	367.15	26.01	26.01
H-	33.23	33.19	26.02	26.01

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
H2	0.00	0.00	31.21	31.21
H2ALME	6.00	6.00	61.73	61.73
H2ASME	24.05	24.05	64.85	64.85
H2C4O	54.58	54.59	66.42	66.43
H2CCC	160.67	160.67	61.07	61.07
H2CCC(S)	133.42	133.42	58.50	58.49
H2CCCCCH	128.19	128.19	75.36	75.37
H2CCCCH	111.34	111.32	72.83	72.94
H2CCCCH2	75.53	75.49	64.77	65.12
H2CCCH	83.03	83.04	61.48	61.48
H2CCCLO	-11.53	-11.54	69.74	69.67
H2CCH(SICL2H)	-66.26	-66.22	84.68	85.71
H2CCH2OH	-4.57	-4.46	69.01	71.17
H2CCHO	3.55	3.51	61.95	61.87
H2CCHSI	97.77	97.77	66.01	65.94
H2CCHSIH	73.54	73.58	66.68	66.79
H2CCHSIH2	58.21	58.21	69.03	68.94
H2CCHSIH3	20.65	20.70	68.95	69.47
H2CLSICH3	-50.13	-50.06	72.04	73.01
H2CLSISICL3	-146.58	-146.56	100.61	101.70
H2CN	59.10	59.11	53.59	53.59
H2CNCH2	56.61	56.53	61.18	61.01
H2CNCH2O	45.02	44.98	68.50	68.38
H2CNCHO	-0.52	-0.56	66.78	66.64
H2CNH	21.89	21.85	54.81	55.45
H2CNNHO	49.78	49.72	67.28	67.10
H2CNNO	58.35	58.36	66.42	66.98
H2CNNO2	33.62	33.64	72.48	73.06
H2CNO	41.46	41.42	61.08	61.01
H2CNO2	36.44	36.47	65.53	65.58
H2CONO	33.07	33.10	68.31	68.54
H2GAET	-2.30	-2.30	83.68	83.68
H2GAME	15.00	15.00	64.85	64.85
H2NF	-6.49	-6.49	54.73	54.72
H2NNO	18.25	18.21	60.27	60.18
H2NO	15.82	15.82	55.69	55.68

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
H2NOH	-12.23	-12.16	56.04	56.17
H2O	-57.80	-57.80	45.11	45.10
H2O(L)	0.00	-68.31	0.00	16.71
H2O(S)	0.00	-69.96	0.00	10.71
H2O2	0.00	-32.53	0.00	55.65
H2S	-4.90	-4.90	49.15	49.14
H2SI(CH3)2	-23.20	-23.08	72.44	73.83
H2SI(CH3)CH2	25.55	25.61	77.77	79.83
H2SI(NH2)2	-37.30	-37.15	71.62	72.38
H2SIC	167.19	167.19	60.31	60.21
H2SICCH	90.95	90.95	66.92	66.80
H2SICH	105.35	105.42	62.48	63.58
H2SICH2	40.75	40.72	59.94	59.85
H2SICH3	33.05	33.11	64.52	65.41
H2SIN	149.19	149.19	59.51	59.51
H2SINH	40.99	40.95	59.90	60.09
H2SINH2	28.03	28.09	65.77	65.79
H2SINH3	23.78	23.85	66.78	66.78
H2SISIH2	62.90	62.87	66.69	66.89
H3ASGAET3	-11.00	-11.00	124.48	124.48
H3ASGAME3	-4.70	-4.70	102.50	102.50
H3CONHO	6.46	6.56	71.67	72.65
H3SIC	147.61	147.61	61.79	61.71
H3SICCH	53.02	53.02	64.11	64.02
H3SICH	92.67	92.67	65.63	66.94
H3SICH2	41.54	41.54	67.62	68.97
H3SICH3	-7.32	-7.25	61.75	62.43
H3SIN	234.59	234.60	56.93	56.93
H3SINH	51.32	51.34	65.52	66.21
H3SISIH	74.91	74.96	67.99	69.32
H3SISIH3	19.11	19.16	68.06	68.06
HALME	27.25	27.25	62.78	62.78
HALME2	-6.73	-6.72	75.32	75.33
HASALME	56.50	56.50	83.68	83.68
HASGAET	69.15	69.15	97.28	97.28
HASGAME	70.00	70.00	87.88	87.88

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
HASME	42.58	42.58	65.90	65.90
HASME2	18.10	18.10	78.45	78.45
HCCCHCCH	134.95	134.95	73.15	73.17
HCCCL	54.95	54.95	57.29	57.29
HCCHCCH	129.91	129.88	68.80	69.06
HCCO	42.44	42.44	60.74	60.73
HCCOH	20.42	20.43	58.69	58.70
HCCSICL2H	-31.76	-31.76	82.04	82.04
HCL	-22.06	-22.06	44.65	44.64
HCL2SICH3	-94.23	-94.16	79.61	80.53
HCL2SISICL2H	-145.25	-145.24	99.80	101.08
HCLCCCLO	-19.42	-19.43	77.51	77.40
HCLCCHO	-6.02	-6.03	70.20	70.09
HCLSI(CH3)2	-68.24	-68.09	81.59	83.53
HCLSI(CH3)CH2	-19.15	-19.06	83.79	86.52
HCLSICH2	2.62	2.59	68.45	68.37
HCLSICH3	-9.10	-9.03	72.91	74.00
HCLSISI	67.05	67.05	71.34	71.34
HCN	31.89	31.89	48.21	48.21
HCNH	66.15	66.10	55.58	55.90
HCNO	38.42	38.43	53.75	53.79
HCO	10.40	10.40	53.67	53.65
HCO+	199.10	199.10	48.59	48.59
HCOOH	-92.57	-92.61	59.32	59.26
HE	0.00	0.00	0.00	30.12
HE+	0.00	568.46	0.00	31.50
HF	-65.14	-65.14	41.51	41.50
HG2BR2(S)	-48.80	-48.80	52.28	52.27
HG2CL2(S)	-63.32	-63.32	46.02	46.00
HG2F2(S)	-116.00	-116.00	38.40	38.39
HG2I2(S)	-28.46	-28.47	57.67	57.66
HGAET	22.90	22.90	83.68	83.68
HGAET2	-2.30	-2.30	100.50	100.50
HGAME	29.00	29.00	65.90	65.90
HGAME2	2.50	2.50	79.50	79.50
HGBR	24.90	24.90	64.88	64.87

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
HGCL2	-34.97	-34.96	70.43	70.43
HGCL2(S)	-55.00	-55.00	34.54	34.53
HGF2	-70.19	-70.18	63.55	63.55
HGF2(S)	-101.00	-101.00	27.80	27.79
HGH	57.00	57.00	52.49	52.48
HGI	31.90	31.90	67.07	67.06
HGO	10.00	10.00	57.13	57.13
HGO(S)	-21.70	-21.70	16.80	16.79
HMEGAET	4.00	4.00	88.90	88.90
HN(OH)2	-24.72	-24.64	61.98	62.09
HN3	71.87	71.87	239.08	57.14
HNC	43.85	43.85	48.93	48.93
HNCN	76.43	76.43	59.36	59.36
HNCNH	35.61	35.71	57.31	57.42
HNCO	-28.22	-28.22	57.05	57.05
HNF	32.00	32.00	54.98	54.97
HNF2	-13.79	-13.79	60.06	60.06
HNNHO	21.91	21.86	58.70	58.63
HNNO	55.25	55.20	60.59	60.53
HNNONO	59.02	58.99	70.98	70.97
HNO	23.80	23.80	52.73	52.72
HNO2	-14.15	-14.15	56.75	56.73
HNO3	-32.10	-32.10	63.66	63.66
HNOH	21.05	21.06	55.78	55.78
HO2	2.50	2.50	54.73	54.72
HOCH2OH	-96.64	-96.53	61.14	61.31
HOCL	-18.64	-18.64	56.34	56.33
HOCN	-3.55	-3.53	57.66	59.25
HOCO	-46.31	-46.29	60.12	60.11
HONO	-18.34	-18.34	59.59	59.58
HONO2	-30.18	-30.18	63.20	63.16
HSI(CH3)2	18.27	18.38	74.81	76.56
HSI(CH3)2CH2	9.32	9.44	86.18	88.89
HSI(CH3)3	-39.40	-39.24	83.61	85.87
HSI(NH2)2	5.62	5.77	72.56	73.38
HSI(NH2)3	-64.86	-64.68	78.65	79.52

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
HSIC	184.85	184.85	58.24	58.13
HSICCH	104.97	104.97	64.44	64.32
HSICH2	85.83	85.81	60.64	60.53
HSICH3	48.84	48.90	62.04	63.21
HSICL	17.00	17.00	59.80	59.80
HSIN	92.99	92.99	54.76	54.75
HSINH	84.80	84.79	60.63	60.68
HSINH2	26.33	26.29	59.77	60.05
HSISICL	79.13	79.11	73.04	72.96
I*C3H7	0.00	18.20	0.00	60.09
K	21.31	21.31	38.30	38.30
K(L)	0.55	0.55	17.08	17.07
K+	122.90	122.90	36.92	36.92
K2	30.37	30.37	59.67	59.66
K2B4O7(S)	-796.90	-796.89	49.80	49.82
K2B6O10(S)	-1107.44	-1107.50	60.00	59.87
K2B8O13(S)	-1420.92	-1420.93	70.20	70.18
K2CO3(S)	-274.90	-274.91	37.17	37.15
K2H2O2	-156.50	-156.50	78.37	78.35
K2O(S)	-86.80	-86.79	22.50	22.51
K2O2(S)	-118.50	-118.47	27.00	27.05
K2SO4	-261.50	-261.50	87.49	87.50
K2SO4(A)	-343.62	-343.62	41.96	41.94
K2SO4(B)	-340.40	-340.41	45.96	45.94
K3CL6AL(S)	-500.00	-499.97	90.00	90.08
K3CL9AL2(S)	-683.60	-683.61	112.00	111.96
K3F6AL(S)	-795.00	-794.96	68.00	68.11
KBF4	-371.00	-371.00	75.35	75.36
KBO2	-161.10	-161.10	71.06	71.06
KBO2(S)	-237.80	-237.81	19.12	19.10
KBR	-43.04	-43.04	59.85	59.85
KBR(L)	-89.98	-89.99	25.23	25.22
KBR(S)	-94.12	-94.12	22.93	22.92
KCL	-51.31	-51.31	57.12	57.11
KCL(L)	-100.81	-100.81	20.71	20.71
KCL(S)	-104.37	-104.37	19.73	19.73

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
KCL4AL(S)	-286.00	-286.01	47.00	46.98
KCLO4(S)	-102.80	-100.21	36.10	40.62
KCN	19.00	19.00	60.48	60.47
KCN(L)	-24.89	-24.89	32.10	32.09
KCN(S)	-27.12	-27.12	30.54	30.53
KF	-78.10	-78.10	54.14	54.13
KF(L)	-132.52	-132.52	16.17	16.16
KF(S)	-135.90	-135.90	15.91	15.91
KH	29.40	29.40	47.30	47.30
KH(S)	-13.82	-13.81	12.00	12.02
KI	-30.00	-30.00	61.70	61.70
KI(L)	-74.77	-74.77	27.27	27.26
KI(S)	-78.37	-78.37	25.43	25.42
KO	17.00	17.00	56.86	56.86
KO-	-33.00	-33.00	54.06	54.06
KO2(S)	-68.00	-68.00	29.28	29.27
KOH	-98.64	-98.65	23.09	23.07
KOH+	119.00	119.00	59.80	59.81
ME2GAET	-5.25	-5.25	97.28	97.28
MEGAET	14.25	14.25	89.95	89.95
MEGAET2	-7.33	-7.32	106.70	106.71
MG	35.28	35.28	35.50	35.50
MG(L)	2.16	2.16	10.16	10.16
MG(S)	0.00	0.00	7.81	7.81
MG+	213.09	213.09	36.88	36.88
MG2	68.91	68.91	58.28	58.27
MG2BR4	-183.50	-183.50	110.24	110.23
MG2C3(S)	19.00	19.00	24.00	24.01
MG2F4	-410.70	-410.69	80.52	80.55
MGAL2O4(S)	-549.50	-549.49	21.20	21.22
MGB2(S)	-21.98	-21.99	8.60	8.59
MGBR	-8.45	-8.45	58.52	58.52
MGBR2	-72.40	-72.40	71.92	71.92
MGBR2+	174.80	174.80	76.87	76.87
MGC2(S)	21.00	21.00	13.00	13.01
MGCL	-10.40	-10.40	55.76	55.76

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
MGCL2	-93.80	-93.80	66.18	66.18
MGCL2(S)	-153.35	-153.35	21.42	21.42
MGCO3(S)	-265.70	-265.70	15.74	15.73
MGF	-56.60	-56.60	52.81	52.81
MGF2	-173.70	-173.70	61.28	61.28
MGF2(S)	-268.70	-268.70	13.68	13.67
MGF2+	141.49	141.49	61.67	61.68
MGH	40.40	40.40	46.15	46.14
MGH2(S)	-18.20	-18.20	7.43	7.42
MGH2O2	-136.80	-136.80	63.85	63.87
MGH2O2(S)	-221.00	-221.00	15.12	15.10
MGN	69.00	69.00	53.71	53.71
MGO(S)	-143.70	-143.70	6.44	6.45
MGOH	-39.38	-39.38	54.10	54.11
MGOH+	139.68	139.68	52.75	52.76
MGS	34.71	34.71	53.87	53.84
MGS(S)	-82.63	-82.63	12.03	12.02
MGSO4(S)	-301.57	-301.58	21.84	21.83
N	112.98	112.95	36.61	36.61
N*C3H7	0.00	22.60	0.00	64.13
N2	0.00	0.00	45.77	45.76
N2F2(C)	17.88	17.88	62.26	62.24
N2F2(T)	20.08	20.07	62.14	62.06
N2F4	-2.00	-2.00	71.96	71.98
N2H2	50.90	50.90	52.22	52.20
N2H3	0.00	36.78	0.00	54.61
N2H4	22.79	22.79	57.03	57.02
N2H4(L)	12.10	12.09	29.05	29.03
N2O	19.61	19.61	52.55	52.55
N2O+	318.69	318.69	55.87	55.86
N2O4	2.17	2.17	72.72	72.72
N3	99.00	99.00	54.10	54.10
NA	25.76	25.75	36.71	36.71
NA(L)	0.58	0.57	13.83	13.82
NA+	145.76	145.75	35.34	35.33
NA2	32.87	32.87	54.99	54.99

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
NA2B4O7(S)	-783.16	-783.17	45.29	45.27
NA2B6O10(S)	-1094.76	-1094.79	55.50	55.43
NA2C2N2	-2.10	-2.10	82.93	82.93
NA2F2	-202.30	-202.30	68.66	68.67
NA2H2O2	-145.20	-145.20	73.44	73.43
NA2O(L)	-89.11	-89.12	21.90	21.88
NA2O(S)	-99.90	-98.48	17.94	19.10
NA2O2	-122.66	-121.57	22.66	24.05
NA2SO4	-247.04	-247.04	82.87	82.89
NA2SO4(D)	-329.66	-329.66	39.01	38.99
NA2SO4(i)	-330.04	-330.04	38.30	38.28
NA2SO4(iii)	-330.99	-330.99	37.02	37.01
NA2SO4(iv)	-331.63	-331.64	35.89	35.87
NA2SO4(v)	-331.70	-331.70	35.75	35.74
NA3CL6AL(S)	-473.00	-472.97	83.00	83.08
NA3F6AL(S)	-792.76	-792.77	57.00	56.97
NABH4(S)	-45.85	-45.85	24.23	24.23
NABO2	-155.00	-155.00	68.63	68.63
NABO2(S)	-233.20	-233.21	17.58	17.56
NABR	-34.40	-34.40	57.63	57.63
NABR(L)	-81.11	-81.11	24.94	24.93
NABR(S)	-86.38	-86.38	20.75	20.74
NACH	22.53	22.53	58.14	58.14
NACL	-43.36	-43.36	54.90	54.90
NACL(S)	-98.26	-98.26	17.24	17.23
NACL4AL(S)	-273.00	-273.01	45.00	44.97
NACN	22.53	22.53	58.14	58.14
NACN(S)	-21.68	-21.68	28.32	28.31
NAF	-69.42	-69.42	51.98	51.98
NAF2-	-160.00	-160.00	59.89	59.89
NAF4AL	-440.00	-440.00	82.41	82.43
NAH	29.70	29.70	45.00	44.99
NAI(S)	-68.80	-68.80	23.54	23.54
NAO	20.00	20.00	54.74	54.74
NAO-	-29.00	-29.00	51.95	51.95
NAO2(S)	-62.30	-62.30	27.70	27.69

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
NAO2AL(S)	-270.84	-270.59	16.83	17.17
NAOH	-47.27	-47.26	54.57	54.58
NAOH(L)	-99.64	-99.64	18.13	18.12
NAOH+	162.00	162.00	57.96	57.96
NCN	107.59	107.59	54.77	54.76
NCO	31.51	31.51	54.14	54.14
NF	53.93	53.93	50.82	50.82
NF2	7.87	7.87	59.40	59.39
NF3	-27.97	-27.97	61.79	61.79
NFO	-15.70	-15.70	59.27	59.27
NFO2	-26.00	-26.00	62.18	62.18
NH	85.20	85.20	43.29	43.29
NH2	45.50	45.50	46.51	46.50
NH3	-10.97	-10.97	46.05	46.03
NNH	58.57	58.57	53.63	53.62
NO	21.58	21.58	50.35	50.34
NO+	236.66	236.66	47.35	47.34
NO2	7.91	7.91	57.34	57.33
NO2-	-48.45	-48.45	56.52	56.51
NO2F	-23.10	-23.09	61.26	61.26
NO3	17.00	17.00	60.35	60.35
NO3F	3.34	3.34	68.94	68.85
NOF	-16.91	-16.90	58.63	58.63
NOF3	-39.00	-39.00	66.54	66.55
O	59.55	59.55	38.47	38.46
O+	374.95	374.95	37.01	37.01
O-	24.32	24.32	37.69	37.68
O2	0.00	0.00	49.01	49.00
O2-	-11.61	-11.62	50.06	50.06
O2F	22.56	22.56	60.57	60.56
O3	34.10	34.10	57.08	57.08
OC(OH)2	-147.04	-147.04	64.46	64.40
OCHCHO	-49.55	-49.53	64.82	64.98
OCHNNHO	-2.05	-2.09	69.36	69.15
OF	23.73	23.73	50.43	50.43
OF2	4.60	4.60	58.54	58.54

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
OH	9.32	9.32	43.88	43.87
OH+	314.80	314.80	43.66	43.65
OH-	-34.32	-34.32	41.19	41.19
ONHNHO	23.55	23.52	62.66	62.55
ONHNOH	-1.77	-1.77	65.04	64.93
P	79.80	79.80	38.98	38.98
P2	42.68	42.68	52.11	52.11
P4	30.77	30.78	66.89	66.92
S	66.20	66.20	40.09	40.09
S(L)	0.00	0.44	0.00	8.77
S(S)	0.00	0.00	0.00	7.62
S+	306.48	306.47	39.08	39.08
S-TRIAZINE	56.36	56.37	64.49	64.49
S2	30.71	30.71	54.51	54.50
SH	33.30	33.30	46.73	46.73
SI	107.70	107.70	40.12	40.12
SI(CH3)2	32.16	32.19	74.55	77.23
SI(CH3)3	3.12	3.28	84.75	87.23
SI(CH3)3CH2	-6.88	-6.71	96.57	99.89
SI(CH3)4	-55.74	-55.51	93.08	96.05
SI(L)	11.59	11.58	10.63	10.62
SI(NH2)3	-18.77	-18.63	84.34	84.27
SI(NH2)4	-92.88	-92.67	84.54	85.38
SI(S)	0.00	0.00	4.50	4.50
SI2	145.79	145.79	54.83	54.83
SI2C	128.00	128.00	57.88	57.88
SI2CL5	-151.65	-151.64	109.12	110.10
SI2CL5H	-188.98	-188.97	108.00	108.98
SI2CL6	-232.75	-232.73	111.13	111.85
SI2F6	-569.62	-569.61	97.16	97.16
SI2H2	95.63	95.62	58.84	58.83
SI2H3	105.70	105.70	65.51	65.51
SI2H5	55.70	55.70	68.85	68.85
SI2H6	19.10	19.10	64.54	64.53
SI3	152.00	152.00	64.00	64.01
SI3H8	28.90	28.90	81.57	81.56

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
SI3N4(A)	-178.00	-178.00	27.00	26.99
SIC	172.00	172.01	50.89	50.93
SIC(B)	-17.50	-17.50	3.97	3.98
SIC2	147.00	147.00	56.55	56.55
SICCH	125.77	125.77	60.40	60.26
SICH	124.39	124.39	54.94	54.83
SICH2	74.15	74.15	55.99	55.92
SICH3	74.53	74.53	60.16	60.13
SICL	37.90	37.90	56.80	56.80
SICL2	-40.30	-40.30	67.20	67.20
SICL2H2	-74.50	-74.50	68.40	68.40
SICL3	-76.50	-76.50	75.50	75.50
SICL3CH2CH	-140.60	-140.59	93.99	95.65
SICL3H	-118.60	-118.60	74.90	74.89
SICL4	-158.40	-158.40	79.10	79.09
SICLH3	-32.20	-32.20	59.80	59.79
SIF	-12.42	-12.42	52.71	52.71
SIF(NH2)2	-95.48	-95.33	76.93	77.70
SIF(NH2)3	-170.70	-170.55	87.97	87.91
SIF2	-149.86	-149.86	61.38	61.38
SIF2(NH2)2	-247.30	-247.19	82.82	82.77
SIF2N	-63.11	-63.11	70.51	70.51
SIF2NH2	-167.24	-167.21	77.17	77.48
SIF3	-237.42	-237.42	67.76	67.76
SIF3NH	-249.65	-249.65	82.15	83.70
SIF3NH2	-317.89	-317.89	79.98	81.03
SIF3NHSIH3	-320.19	-320.16	95.97	96.88
SIF3NSIH3	-252.84	-252.83	97.65	99.34
SIF4	-385.98	-385.98	67.55	67.54
SIFH3	-85.50	-85.50	57.00	57.00
SIFNH	-13.57	-13.49	68.88	68.95
SIFNH2	-80.01	-80.04	64.68	64.62
SIH	91.70	91.70	44.20	44.20
SIH2	64.80	64.80	49.50	49.49
SIH2CL	7.80	7.80	62.30	62.30
SIH2F	-42.16	-42.16	59.70	59.70

Table A.1 Standard State Enthalpies and Entropies at 298 K. (continued)

Species	$H^0(298)$ (Kcal/mol)		$S^0(298)$ (cal/mol-K)	
	Data	Fit	Data	Fit
SIH2F2	-186.38	-186.38	62.81	62.81
SIH3	47.43	47.43	51.81	51.80
SIH3NH2	-11.45	-11.40	65.66	65.66
SIH3NHSIH3	-14.32	-14.32	83.54	85.95
SIH3NSIH3	48.90	48.90	83.75	86.69
SIH3SIH2CH3	4.03	4.14	79.43	81.90
SIH4	8.09	8.10	48.90	48.90
SIHCL2	-34.30	-34.30	70.30	70.30
SIHF	-35.70	-35.70	57.07	57.07
SIHF2	-139.57	-139.57	65.05	65.05
SIHF3	-288.63	-288.63	66.65	66.65
SIN	115.55	115.55	51.95	51.95
SINH	38.39	38.39	51.66	51.66
SINH2	48.67	48.67	58.56	58.56
SN	63.00	63.00	53.06	53.05
SO	1.20	1.20	53.02	53.01
SO2	-70.95	-70.95	59.30	59.29
SO3	-94.59	-94.59	61.34	61.34
TI	113.20	113.20	43.07	43.06
TICL	36.90	36.90	59.54	59.54
TICL2	-56.70	-56.70	66.50	66.50
TICL3	-128.90	-128.90	75.70	75.71
TICL4	-182.40	-182.40	84.79	84.80

Appendix B. Database Listing in the CHEMKIN Format

CHEMKIN expects that the thermodynamic data is in a specific format, which is essentially the same as that used by the NASA Complex Chemical Equilibrium Program.[13] In addition to the fourteen fit coefficients, the database also contains the species' name, its elemental composition, its electronic charge, and an indication of its phase (gas, solid, liquid or solid). The data for each species requires four formatted records of length 80 characters. Table B.1 is a sample of the records and Table B.2 provides a detailed specification of the format for the "therm.dat" file. The first two lines in Table B.1 are required at the top of a "therm.dat" file; the first line specifies that the following is a set of thermodynamic data, while the second line provides the three temperatures used in the fitting process (a low temperature, break temperature, and high temperature). The user must also adhere to these specifications when placing thermodynamic data within the input file read by the CHEMKIN Interpreter.

An alternative input data format allows specification of more than two temperature ranges. Use of this format is not backwards-compatible with the old NASA format, but does provide more flexibility in describing the thermodynamic data for complex functions of temperature. This alternative approach is summarized at the end of Table B.2. The alternative lines 7-9 can be used in place of lines 4 - 6. Lines 7 specifies all of the temperature values that define the temperature intervals. Lines 8-9 are then repeated for each specified temperature interval, in **descending** order of temperature ranges.

Table B.1 Excerpts from the CHEMKIN Thermodynamic Data File

```
THERMO
   300.000  1000.000  5000.000
(CH2O)3            70590C   3H   6O   3     G  0300.00   4000.00  1500.00      1
 0.01913678E+03 0.08578044E-01-0.08882060E-05-0.03574819E-08 0.06605142E-12    2
-0.06560876E+06-0.08432507E+03-0.04662286E+02 0.06091547E+00-0.04710536E-03    3
 0.01968843E-06-0.03563271E-10-0.05665403E+06 0.04525264E+03                   4
AL                 62987AL  1               G  0300.00   5000.00  0600.00      1
 0.02559589E+02-0.10632239E-03 0.07202828E-06-0.02121105E-09 0.02289429E-13    2
 0.03890214E+06 0.05234522E+02 0.02736825E+02-0.05912374E-02-0.04033937E-05    3
 0.02322343E-07-0.01705599E-10 0.03886794E+06 0.04363879E+02                   4
END
```

Table B.2 Format of the Species Data in the CHEMKIN Thermodynamic Data File ("therm.dat")

Record Number	Contents	Format	Column Number
1	Species names (Must start in Column 1)	18A1	1 - 18
	Date (Not used in the program)	6A1	19 - 24
	Atomic symbols and formula	4(2A1,I3)	25 - 44
	Phase of species (S, L, or G for solid, liquid or gas)	A1	45
	Low Temperature	E10.0	46 - 55
	High Temperature	E10.0	56 - 65
	Common temperature (If needed, blank for default)	E8.0	66 - 73
	Atomic symbols and formula (Blank for default)	2A1,I3	74 - 78
	The integer "1"	I1	80
	Atomic symbols and formula (Blank for default)	2(2A1,I3)	81 -100
2	Coefficients a_1 - a_5 in polynomial fit for the upper temperature interval	5(E15.8)	1 - 75
	The integer "2"	I1	80
3	Coefficients a_6 - a_7 for the upper temperature interval, and a_1, a_2, and a_3 for the lower temperature range	5(E15.8)	1 - 75
	The integer "3"	I1	80
4	Coefficients a_4, a_5, a_6, a_7 for the lower temperature range	4(E15.8)	1 – 60
	The integer "4"	I1	80
Alternative lines for more than 2 temperature intervals (in place of Lines 4-6 above):			
7	TEMP followed by space-delimited minimum fit temperature, common temperatures in increasing order, and maximum fit temperature	A4, Free	1 to 80
8	Coefficients a_1 - a_5 for a temperature interval	5(E15.8)	1 to 75
9	Coefficients a_6, a_7 for a temperature interval	2(E15.8)	1 to 30

Appendix C. Graphical Representation of the Database

Figure C.1 shows a graphical representation of the polynomial fits to the specific heat c_P/R, enthalpy H^0/RT, and entropy S^0/R, a typical example. The fitting procedure and functional form of the polynomials are discussed in more detail in Chapter 3. Figure C.1 shows the features of the graphical comparisons of the fitted polynomial representations of the thermodynamic data with the original experimental or calculated values. The remaining pages of this Appendix include such comparisons for all the species included in the CHEMKIN Thermodynamic Database File ("therm.dat").

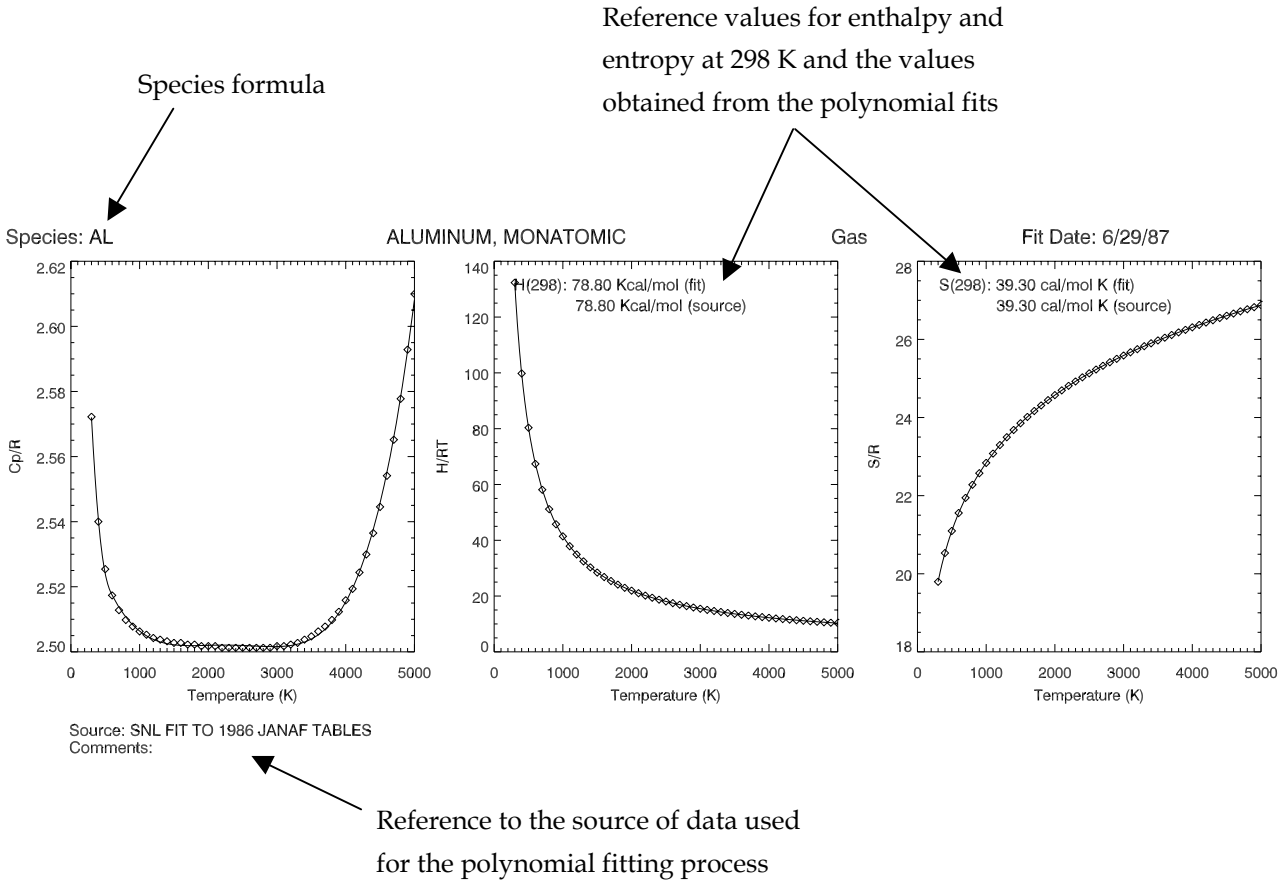

Figure C.1 A sample plot of the temperature variation of the specific heat, enthalpy and entropy for Aluminum annotated with explanatory notes