

Coefficients for Calculating Thermodynamic and Transport Properties of Individual Species

Bonnie J. McBride
Lewis Research Center
Cleveland, Ohio

Sanford Gordon
Sanford Gordon and Associates
Cleveland, Ohio

Martin A. Reno
Heidelberg College
Tiffin, Ohio

NASA
National Aeronautics and
Space Administration
Office of Management
Scientific and Technical
Information Program

1993

Contents

	Page
Summary	1
Introduction	1
Symbols	2
Standard States, Reference States, and Fundamental Constants	2
Empirical Equations for Fitting Thermodynamic Functions	3
Assigned Enthalpy Values	3
Heats of Formation and Equilibrium Constants	3
Least-Squares Fit	3
Thermodynamic Data Coefficients	4
Names	4
Heats of Formation	4
Six-Character Reference Codes	4
Atomic Symbols in Formula Used by CETPC and CET89	4
Phase and Species Order	5
Temperature Ranges	5
Coefficients	5
Transport Property Coefficients	5
Concluding Remarks	5
References	5
Table I.—Format for Thermodynamic Data Coefficients in Table II	9
Table II.—Thermodynamic Data Coefficients	10
Table III.—Format for Transport Property Data in Table IV	74
Table IV.—Transport Property Coefficients	75

Summary

Libraries of thermodynamic data and transport properties are given for individual species in the form of least-squares coefficients. Values of heat capacity $C_p^o(T)$, enthalpy $H^o(T)$, and entropy $S^o(T)$ are available for 1130 solid, liquid, and gaseous species. Viscosity and thermal conductivity data are given for 155 gases. The original $C_p^o(T)$ values were fit to a fourth-order polynomial with integration constants for $H^o(T)$ and $S^o(T)$. For each species the integration constant for $H^o(T)$ includes the heat of formation. Transport properties have a different functional form. The temperature range for most of the data is 300 to 5000 K, although some of the newer thermodynamic data have a range of 200 to 6000 K. Because the species are mainly possible products of reaction, the data are useful for chemical equilibrium and kinetics computer codes. Much of the data has been distributed for several years with the NASA Lewis equilibrium program CET89. The thermodynamic properties of the reference elements have been updated along with about 175 species that involve the elements carbon, hydrogen, oxygen, and nitrogen. These sets of data will be distributed with the NASA Lewis personal computer program for calculating chemical equilibria, CETPC.

Only the executable code will be included and the coefficient data will be unformatted and not legible. This report lists these thermodynamic and transport coefficients in a legible formatted form and gives data references. These data bases will also be available on diskettes in the formatted form and will be included with future distributions of the CET89 source code.

The functional form for $C_p^o(T)$ is a fourth-order polynomial with integration constants for $H^o(T)$ and $S^o(T)$. Much of the coefficient data are the same as the data that have been distributed for several years with the NASA Lewis equilibrium program CET89 except that they have been adjusted for newer physical constants (Cohen and Taylor, 1987), for newer atomic weights (De Laeter and Heumann, 1991), and for the reference pressure for the ideal gases as 1 bar rather than 1 atmosphere. Some data have been updated. These include the reference elements (McBride et al., 1993) and about 175 species that involve the elements carbon, hydrogen, oxygen, and nitrogen. Generally, these newer data were calculated by using PAC91 (McBride and Gordon, 1992), and the older data were calculated by using earlier versions of that code. The coefficients for the older data are for the temperature intervals 300 to 1000 K and 1000 to 5000 K. The fits were constrained so that the coefficient functional form gives results that match the original data at 1000 K. The coefficients for the newer data are for the intervals 200 to 1000 K and 1000 to 6000 K. The fits were constrained so that the functional form values match the original data at 298.15 K and also so that the higher interval functional values match the lower interval functional values at 1000 K.

The original data for gases are generally the result of ideal-gas calculations, whereas the data for the condensed species are generally the result of a fit to experimental measurements. For most species either the thermodynamic functions or the molecular constant data are taken from other compilations such as JANAF (Chase et al., 1985) and the Russian volumes (Gurvich et al., 1978, 1979, 1982, 1989, and 1991), although many other references were used.

The transport property data from which the least-squares coefficients were generated are described in Gordon et al. (1984). Coefficients are given for viscosity, thermal conductivity, and three binary viscosity interactions. The functional form to which the data are fitted is described in a later section. The temperature range was divided into two intervals, 300 to 1000 K and 1000 to 5000 K. This corresponds to the

Introduction

This report documents the thermodynamic and transport property data used in several versions of the NASA Lewis equilibrium computer programs CET89 (Gordon et al., 1971, 1976, 1984, and 1988) and CETPC (to be published). Many other computer codes, such as the one given in Radhakrishnan and Bittker (1993), use the same data. The libraries of data are presented in the form of least-squares coefficients. Thermodynamic data coefficients are given for 1130 species (gaseous, liquid, or solid). Transport property coefficients are given for 155 gaseous species. These coefficients generate the thermodynamic functions heat capacity $C_p^o(T)$, enthalpy $H^o(T)$, and entropy $S^o(T)$ and the transport properties viscosity η and thermal conductivity λ .

CETPC is essentially CET89 adapted for use on an IBM-compatible personal computer. This code, the accompanying thermodynamic and transport property coefficients, and sample problems will be distributed on a 3½-in. diskette.

temperature intervals used for the thermodynamic data at the time of the Gordon et al. (1984) report.

The data are presented in the form required by CET89 and CETPC and are annotated with the references.

Symbols

a_i	polynomial coefficients used in eqs. (1) to (3)
b_1	integration constant defined by eq. (2)
b_2	integration constant defined by eq. (3)
$C_p^o(T)$	heat capacity at constant pressure for standard state
c	speed of light
c_2	second radiation constant, hc/k
$G^o(T)$	either $\{G^o(T) - H^o(0)\} + H^o(0)$ or $\{G^o(T) - H^o(298.15)\} + H^o(298.15)$
$G^o(T) - H^o(0)$	Gibbs energy at temperature T relative to enthalpy at 0 K for standard state
$G^o(T) - H^o(298.15)$	Gibbs energy at temperature T relative to enthalpy at 298.15 K for standard state
$\Delta_f G^o(T)$	Gibbs energy of formation of a substance at temperature T from its reference elements in their standard state
$H^o(0)$	chemical energy at 0 K for standard state
$H^o(298.15)$	assigned enthalpy at 298.15 K for standard state (assigned to be equal to $\Delta_f H^o(298.15)$)
$H^o(T)$	either $\{H^o(T) - H^o(0)\} + H^o(0)$ or $\{H^o(T) - H^o(298.15)\} + H^o(298.15)$
$H^o(T) - H^o(298.15)$	sensible enthalpy at temperature T relative to 298.15 K for standard state
$\Delta_f H^o(T)$	enthalpy of formation (heat of formation) of a substance at temperature T from its reference elements in the standard state
h	Planck's constant
K	equilibrium constant
k	Boltzmann constant
m_e	electron mass
N	principal quantum number for atomic species
p_0	standard-state pressure
q_i	temperature exponents in eq. (1)
R	universal gas constant

r	number of coefficients a_i in eq. (1)
S_o/R	Sackur-Tetrode constant
$S^o(T)$	entropy at temperature T for standard state
T	temperature, K
η	viscosity, eq. (10)
λ	thermal conductivity, eq. (10)

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 states. For gases this is ideal gas at the standard pressure of 10^5 Pa (1 bar). For condensed species the standard state is the pure crystalline or liquid substance at the same standard pressure. All thermodynamic properties are standard molar quantities.

The reference states of the elements as well as the data used for these elements are given in McBride et al. (1993). Generally they are taken to be the thermodynamically stable state at 298.15 K. For those species that are gases at 298.15 K and 1 bar, the entire temperature range is taken to be gaseous. For species that are condensed at 298.15 K the entire range is taken to be condensed with transitions between various phases, such as between solid and liquid phases.

Most of the properties are given in the International System of Units (SI); that is, the temperatures are in kelvin (K), the energies in joules (J), and the pressures in bars. Sometimes the values are made dimensionless by dividing them either by the gas constant R or RT . The fundamental constants were taken from Cohen (1987) and are as follows:

Quantity	Symbol	Value	Units
Molar gas constant	R	8.314510(70)	J/(mol·K)
Sackur-Tetrode constant: For $p_0=100\ 000$ Pa =1 bar	S_o/R	-1.151693(21)	
For $p_0=101\ 325$ Pa =1 atm	S_o/R	-1.64856(21)	
Second radiation constant, hc/k	c_2	0.01438769(12)	mK
Electron mass	m_e	0.000548579903(13)	^a u

^aAtomic mass unit used for calculating molar masses, $1/12$ mass ^{12}C .

These constants were used in McBride and Gordon (1992) in calculating the thermodynamic functions for many gases. The atomic weights were taken from De Laeter and Heumann (1991). These weights are given in atomic mass units (u) based on $^{12}\text{C} = 12\text{u}$. Some of the older data were calculated with values of R , Sackur-Tetrode constants, and atomic weights

different from those selected for this report. The coefficients were corrected to adjust for the differences in these values.

Empirical Equations for Fitting Thermodynamic Functions

The thermodynamic data for many individual species can be conveniently stored for use with computer programs in the form of coefficients associated with equations that fit the data. The following dimensionless form was chosen for this report:

$$\frac{C_p^o(T)}{R} = \sum_{i=1}^r a_i T^{q_i} \quad (1)$$

For CET89 and CETPC, $r = 5$ and the q_i values are 0, 1, 2, 3, and 4. A second set is planned for future NASA Lewis chemical equilibrium codes. The new set has two additional terms ($r = 7$), one with $q_i = -1$ and one with $q_i = -2$. (See the section Least-Squares Fit for an additional discussion of these equations.)

Enthalpy and entropy are related thermodynamically to $C_p^o(R)$ as follows:

$$\frac{H^o(T)}{RT} = \frac{b_1}{T} + \frac{\int C_p^o(T) dT}{RT} \quad (2)$$

$$\frac{S^o(T)}{R} = b_2 + \int \left(\frac{C_p^o(T)}{RT} \right) dT \quad (3)$$

where b_1 and b_2 are integration constants. These are two additional constants (or coefficients) to the five or seven coefficients in equation (1).

These equations are given again in table I along with the format of the data listed in table II.

Assigned Enthalpy Values

For some applications, such as those discussed in Gordon and McBride (1976), it is convenient to combine sensible enthalpies and energies of chemical and physical changes into one numerical value. An arbitrary base may be adopted for assigning absolute values to the enthalpy of various substances inasmuch as only differences in enthalpies are measurable. For CET89 and CETPC the arbitrary base selected was a value of zero at 298.15 K for the reference elements. Thus, for the assigned reference elements

$$\Delta_f H^o(298.15) = H^o(298.15) = 0 \quad (4)$$

And, in general, for all species

$$H^o(298.15) = \Delta_f H^o(298.15) \quad (5)$$

$$H^o(T) = H^o(298.15) + \{H^o(T) - H^o(298.15)\} \quad (6)$$

Heats of Formation and Equilibrium Constants

Heats of formation and $\log_{10}K$ for a species are calculated as a function of temperature for the formation of the species from the elements in their assigned reference states. The following is an example of how these properties can be calculated for CO(g) at 1000 K

$$\begin{aligned} \Delta_f H^o(1000) &= H^o(1000)CO(g) - H^o(1000)C(gr) \\ &\quad - \frac{1}{2} H^o(1000) O_2(g) \end{aligned} \quad (7)$$

$$\begin{aligned} \Delta_f G^o(1000) &= G^o(1000)CO(g) - G^o(1000)C(gr) \\ &\quad - \frac{1}{2} G^o(1000) O_2(g) \end{aligned} \quad (8)$$

By definition,

$$\log_{10} K = \frac{-\Delta_f G^o(T)}{2.3025851 RT} \quad (9)$$

Least-Squares Fit

For most of the species in this report the coefficients in equations (1) to (3) were obtained by means of a least-squares fit. The code PAC91 (McBride and Gordon, 1992) and earlier versions of the code (e.g., McBride and Gordon, 1967) were used to obtain the coefficients. For all calculations (1) a fourth-order polynomial was used for $C_p^o(T)$; (2) the temperature range was split into two intervals with a breakpoint at 1000 K; (3) a fitting constraint required coefficients in both intervals to yield the same values of the functions at the 1000 K common point; and (4) generally the functions $C_p^o(T)/R$, $H^o(T)/R$, and $S^o(T)/R$ were fit simultaneously (Zeleznik and Gordon, 1961).

There are two major differences between the data produced by PAC91 and the data produced by earlier PAC versions: the overall temperature range and the point where the coefficients reproduce the original functions exactly. Generally, the PAC91 data are for the range 200 (or 298.15 for ions) to 6000 K, whereas the older data are for the range 300 to 5000 K. The exact-fit points are 1000 K for the older data and 298.15 K for the newer data. Thus, the newer data reproduce the heats of formation exactly at 298.15 K.

Thermodynamic functions for some gases were not recalculated but rather taken directly from tables. When these data do not cover the entire temperature range used here, they must be extrapolated before they are fit. Data for the entire range is a requirement of equilibrium programs such as CETPC and CEA (Gordon and McBride, 1993). Although many of these species are not expected to exist at these high temperatures, the program includes the species at the higher temperature and then uses the coefficient data to decide whether the species should be included. If the data are fit to some temperature much lower than the 5000 or 6000 K limit, the coefficients could represent the data so poorly that an incorrect exclusion or inclusion of the species could result. Functions for these species were extrapolated by using the procedure described in Wilhoit (1975). A more complete discussion of this method, as well as the dangers of using coefficients to extrapolate outside of their temperature ranges, is given in McBride and Gordon (1992).

For the condensed species, each phase has its own set of coefficients. When phase transitions occur, the fit was constrained so that the difference in Gibbs energy is zero between the phases.

For some species and some temperature intervals, however, coefficients were not obtained by means of the PAC programs. The exceptions were when the original reference had equations in acceptable form or when $C_p^o(T)$ for an entire temperature interval was constant.

Thermodynamic Data Coefficients

The format of the thermodynamic data coefficients is detailed in table I and the data are listed in table II. In table II the data references are given in a column to the right of the data records. Some further comments are given in the following sections.

Names

Species names are the first 15 characters in the first record for each set. Many of the species names listed here are different from the names used in the data distributed with previous CET89 computer programs. This difference is important when using CET89 and CETPC because the names used in some of the input must be exactly the same as the names used in the thermodynamic data. Older species names were all upper case. The newer names have some lower case characters and the names are case sensitive. The letter "L" is always upper case in the formula part of the name so that it will not be confused with the number "1." Thus, for example, chlorine is given as CL rather than Cl. Various letters are used to represent the solid phases depending on what they were called in the original reference and what FORTRAN characters are available. The following chart shows the meaning of some of the abbreviations:

Abbreviation	Phase
an	andalusite
caL	calcite
cr	crystal
gr	graphite
hqz	high quartz
L	liquid
Lqz	low quartz
rd	red
ru	rutile
yw	yellow
a	alpha
b	beta
c	gamma
d	delta

Heats of Formation

The last floating-point number in each species set is the heat of formation at 298.15 K divided by R . These values are the result of using the coefficients in equation (2). The newer data, generally with temperature ranges from 200 to 298.15 to 6000 K, were forced to fit the original data at 298.15 K. Thus, these heats of formation should match the original values exactly. The older data, however, were forced to fit at 1000 K. Thus, these heats of formation at 298.15 K will be slightly different than the original values.

Six-Character Reference Codes

The second field of the first record contains a six-character reference code to indicate the major source and date of the data. The letters indicate the reference, and the numbers that follow indicate a date. The following chart gives the references associated with the various letter codes.

Letters	References
J	[JANAF] Chase et al. (1985) with date from individual sheet
CODA	[CODATA] Cox et al. (1989)
L	[Lewis] A combination of references or a NASA Lewis reference with date of least-squares fit
TPIS	[Thermodynamic Properties of Individual Substances] Gurvich et al. (1979, 1982, 1989, or 1991)
X	[TeXas] TRC data with date from individual sheet
SRD	[Standard Reference Data] Alcock et al. (1993)
BUR	[Burcat] Burcat et al. (1979, 1982, 1984, 1992)
BAR	[Barin] Barin and Knacke (1973) or Barin et al. (1989)

Atomic Symbols in Formula Used by CETPC and CET89

The atomic symbols used in the chemical formula following the six-character code are the same as those used within the computer programs. The letters are all upper case. The letter "E" represents electrons for the ionized species.

Phase and Species Order

The phase column for the first record of each species indicates whether the species is condensed (C) or gaseous (G). For CET89 and CETPC the order of the sets of data for the gaseous species is immaterial. For the condensed species the data for the various phases must be adjacent and in the order of increasing temperature range. In table II all the gases precede the condensed species. This same order is used within CETPC and CET89.

Temperature Ranges

The temperature ranges listed give the range where the data were fitted. Most of the gases were fitted for the whole range (i.e., 200, 298.15, or 300 K to 5000 or 6000 K). As discussed previously the fits are for two intervals with a common break at 1000 K. The ranges for the condensed species vary according to the original data. For liquids with a constant C_p^o the range is extended to 5000 or 6000 K. Generally, using the coefficients to extrapolate more than a short range outside these limits can result in very large errors. CET89 and CETPC allow the data to be extrapolated 20 percent outside the fitted range.

Coefficients

Records 2, 3, and 4 list the coefficients as indicated in table I. Note that the first seven coefficients are for the higher temperature range and the second seven coefficients are for the lower temperature range.

Transport Property Coefficients

The generation of the transport property coefficients used in this report was discussed in Gordon et al. (1984). Coefficients are given for 155 species. The data used to generate the coefficients were taken from Gordon et al. (1984) for 17 species; the remainder of the data were taken from Svehla (1962).

Transport property coefficients are given for viscosity, thermal conductivity, and for a few pairs of species, a viscosity interaction parameter η_{ij} . The coefficients were generated by a least-squares fit to the following form:

$$\left. \begin{array}{l} \ln \eta \\ \ln \lambda \\ \ln \eta_{ij} \end{array} \right\} = A \ln T + \frac{B}{T} + \frac{C}{T^2} + D \quad (10)$$

These coefficients were generated to give viscosity in units of micropoise (μP) and thermal conductivity in units of microwatts per centimeter kelvin ($\mu W/cm \cdot K$). Coefficients were generated for two temperature intervals, 300 to 1000 K

and 1000 to 5000 K, to be consistent with the thermodynamic data intervals. Each pure species, therefore, has four sets of coefficients: two sets for viscosity (low- and high-temperature intervals) and two sets for thermal conductivity (low- and high-temperature intervals). Only two sets of coefficients are given for the viscosity interactions. The format used for the transport property data is given in table III and the coefficients are given in table IV.

Concluding Remarks

The thermodynamic data for the next NASA Lewis chemical equilibrium program (Gordon and McBride, 1993) will have a different format with the possibility of two additional coefficients in equation (1) and more temperature intervals. For gases there may be as many as three intervals, namely 200 to 1000 K, 1000 to 6000 K, and 6000 to 20 000 K. For condensed species there may be any number of intervals and the breakpoints may be variable (see McBride and Gordon, 1992; and McBride et al., 1993).

References

- Alcock, C.B., Chase, M.W., and Itkin, V., 1993, "Thermodynamic Properties of the Group IIA Elements," *Journal of Physical and Chemical Reference Data*, Vol. 22, No. 1, pp. 1-85.
- Anderson, W.R., 1989, "Oscillator Strengths of NH_2 and the Heats of Formation of NH and NH_2 ," *Journal of Physical Chemistry*, Vol. 93, pp. 530-536.
- Barin, I., and Knacke, O., 1973, *Thermochemical Properties of Inorganic Substances*, Vol. I, Springer-Verlag, New York.
- Barin, I., Sauert, F., Schultze-Rhonhof, E., and Sheng, W.S., 1989, *Thermochemical Data on Pure Substances*, Pt. 1, VCH Publishers, Wiesbaden, Germany.
- Blankenship, F.A., and Belford, R.L., 1962, New York, "VCl₄ Vapor Spectrum and Jahn-Teller Splitting," *Journal of Chemical Physics*, Vol. 36, No. 3, pp. 633-639.
- Bondybey, V.E., and English, J.H., 1977, "Spectroscopy and Vibrational Relaxation of CNN in Rare Gas Solids," *Journal of Chemical Physics*, Vol. 67, No. 2, pp. 664-668.
- Brix, P., and Herzberg, G., 1954, "Fine Structure of the Schumann-Runge Bands Near the Convergence Limit and the Dissociation Energy of the Oxygen Molecule," *Canadian Journal of Physics*, Vol. 32, pp. 110-135.
- Bjarnov, E., Christensen, D.H., and Nielsen, O.F., 1974, "Vibrational Spectra and Force Field of Triacetylene," *Spectrochimica Acta*, Vol. 30A, pp. 1255-1262.
- Brouwer, L.D., Muller-Markgraf, W., and Troe, J., 1988, "Thermal Decomposition of Toluene: A Comparison of Thermal and Laser-Photochemical Activation Experiments," *Journal of Physical Chemistry*, Vol. 92, pp. 4905-4914.

- Bunker, P.R., and Jensen, P., 1983, "A Refined Potential Surface for the \tilde{x}^3B_1 Electronic State of Methylene CH₂," *Journal of Chemical Physics*, Vol. 79, No. 3, pp. 1224-1228.
- Burcat, A., and Kudchadker, S., 1979, "Ideal Gas Thermodynamic Properties for CH₃O and CH₂OH Radicals," *Acta Chimica Academiae Scientiarum Hungaricae*, T. 101, No. 3, pp. 249-258.
- Burcat, A., Miller, D., and Gardiner, W.C., 1982, *Ideal Gas Thermodynamic Properties, Pt. III: C₂H_nO Radicals*, TAE 504, Technion Israel Institute of Technology, Haifa, Israel.
- Burcat, A., 1984, *Thermochemical Data for Combustion Calculations*, Combustion Chemistry, Chapt. 8, W.C. Gardiner, Jr., ed., Springer-Verlag, New York.
- Burcat, A., Zeleznik, F.J., and McBride, B.J., 1985, "Ideal Gas Thermodynamic Properties for the Phenyl, Phenoxy, and o-Biphenyl Radicals," NASA TM-83800.
- Burcat, A., and McBride, B., 1992, *Ideal Gas Thermodynamic Data for Compounds Used in Combustion and Air-Pollution*, TAE 675, Technion Israel Institute of Technology, Haifa, Israel.
- Butcher, R.J., and Jones, W.J., 1973a, "Cyclopropane: Studies of Some Vibration-Rotation Raman Bands," *Journal of Molecular Spectroscopy*, Vol. 47, pp. 64-83.
- Butcher, R.J., and Jones, J., 1973b, "The Raman Spectrum of Allene," *Journal of Raman Spectroscopy*, Vol. 1, pp. 393-414.
- Chao, J., Wilhoit, R.C., and Zwolinski, B.J., 1973, "Ideal Gas Thermodynamic Properties of Ethane and Propane," *Journal of Physical and Chemical Reference Data*, Vol. 2, No. 2, pp. 427-437.
- Chao, J., Rodgers, A.S., Wilhoit, R.C., and Zwolinski, B.J., 1974, "Ideal Gas Thermodynamic Properties of Six Chloroethanes," *Journal of Physical and Chemical Reference Data*, Vol. 3, No. 1, pp. 141-162.
- Chao, J., and Zwolinski, B.J., 1975, "Ideal Gas Thermodynamic Properties of Ethylene and Propylene," *Journal of Physical and Chemical Reference Data*, Vol. 4, No. 1, pp. 251-261.
- Chao, J., and Zwolinski, B.J., 1978, "Ideal Gas Thermodynamic Properties of Methanoic and Ethanoic Acids," *Journal of Physical and Chemical Reference Data*, Vol. 7, No. 1, pp. 363-377.
- Chao, J., Hall, K.R., Marsh, K.N., and Wilhoit, R.C., 1986, "Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C₁ to C₄. Part 2: Ideal Gas Properties," *Journal of Physical and Chemical Reference Data*, Vol. 15, No. 4, pp. 1369-1436.
- Chase, M.W., Jr., ed., 1985, *JANAF Thermochemical Tables*, 3rd ed., Pts. 1 & 2. (*Journal of Physical and Chemical Reference Data*, Vol. 14, Suppl. 1, 1985).
- Chen, S.S., Wilhoit, R.C., and Zwolinski, B.J., 1975, "Ideal Gas Thermodynamic Properties and Isomerization of n-Butane and Isobutane," *Journal of Physical and Chemical Reference Data*, Vol. 4, No. 4, pp. 859-869.
- Chen, S.S., Wilhoit, R.C., and Zwolinski, B.J., 1976, "Ideal Gas Thermodynamic Properties of Six Chlorofluoromethanes," *Journal of Physical and Chemical Reference Data*, Vol. 5, No. 3, pp. 571-580.
- Chen, S.S., Wilhoit, R.C., and Zwolinski, B.J., 1977, "Thermodynamic Properties of Normal and Deuterated Methanols," *Journal of Physical and Chemical Reference Data*, Vol. 6, No. 1, pp. 105-112.
- Chen, Y., Jonas, D.M., Kinsey, J.L., and Field, R.W., 1989, "High Resolution Spectral Cross Correlation," *Journal of Chemical Physics*, Vol. 91, No. 7, pp. 3976-3987.
- Chen, Y., Rauk, A., and Tschiukow-Roux, E., 1990, "Structures, Barriers for Rotation and Inversion, Vibrational Frequencies, and Thermodynamic Functions of Ethyl, Alpha-Fluoroethyl, and Alpha-Difluoroethyl Radicals: An Ab Initio Study," *Journal of Chemical Physics*, Vol. 93, No. 2, pp. 1187-1195.
- Cohen, E.R., and Taylor, B.N., 1987, "The 1986 CODATA Recommended Values of the Fundamental Physical Constants," *National Bureau of Standards, Journal of Research*, Vol. 92, No. 2, pp. 85-95.
- Corliss, C., and Sugar, J., 1979, "Energy Levels of Potassium, K I through K XIX," *Journal of Physical and Chemical Reference Data*, Vol. 8, No. 4, pp. 1109-1145.
- Cox, J.D., 1982, "Notation for States and Processes, Significance of the Word STANDARD in Chemical Thermodynamics, and Remarks on Commonly Tabulated Forms of Thermodynamic Functions," *Pure Applied Chemistry*, Vol. 54, No. 6, pp. 1239-1250.
- Cox, J.D., Wagman, D.D., and Medvedev, V.A., 1989, *CODATA Key Values for Thermodynamics*, Hemisphere Pub. Corp., New York.
- Creighton, J.A., Green, J.H.S., and Kynaston, W., 1966, "The Far-Infrared Spectra and Thermodynamic Properties of Vanadium and Titanium Tetrachlorides," *Journal of Chemical Society, (A)*, pp. 208-210.
- De Laeter, J.R., and Heumann, K.G., 1991, "Atomic Weights of the Elements 1989," *Journal of Physical and Chemical Reference Data*, Vol. 20, No. 6, pp. 1313-1325.
- Dorofeeva, O.V., Gurvich, L.V., and Jorish, V.S., 1986, "Thermodynamic Properties of Twenty-one Monocyclic Hydrocarbons," *Journal of Physical and Chemical Reference Data*, Vol. 15, No. 2, pp. 437-464.
- Dorofeeva, O.V., and Gurvich, L.V., 1991, "Thermodynamic Properties of Linear Carbon Chain Molecules With Conjugated Triple Bonds," *Thermochimica Acta*, Vol. 178, pp. 273-286.
- Douglas, A.E., and Moller, C.K., 1955, "The Predissociation Energy of C¹²O and C¹³O Molecules," *Canadian Journal of Physics*, Vol. 33, No. 3, pp. 125-132.
- Ervin, K.M., Gronert, S., Barlow, S.E., Gilles, M.K., Harrison, A.G., Bierbaum, V.M., DePuy, C.H., Lineberger, W.C., and Ellison, G.B., 1990, "Bond Strengths of Ethylene and Acetylene," *Journal of American Chemical Society*, Vol. 112, pp. 5750-5759.
- Fegley, M.B., Jr., 1981, "The Thermodynamic Properties of Silicon Oxynitride," *Communications of American Ceramic Society*, pp. C124-C126.
- Gibson, S.T., Greene, J.P., and Berkowitz, J., 1985, "Photoionization of the Amidogen Radical," *Journal of Chemical Physics*, Vol. 83, No. 9, pp. 4319-4328.
- Gordon, S., and McBride, B.J., 1971, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," NASA SP-273.
- Gordon, S., and McBride, B.J., 1976, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations," NASA SP-273, Interim Revision.

- Gordon, S., 1982, "Thermodynamic and Transport Combustion Properties of Hydrocarbons With Air, I—Properties in SI Units," NASA TP-1906.
- Gordon, S., McBride, B.J., and Zeleznik, F.J., 1984, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications, Supplement I—Transport Properties," NASA TM-86885.
- Gordon, S., and McBride, B.J., 1988, "Finite Area Combustor Theoretical Rocket Performance," NASA TM-100785.
- Gordon, S., and McBride, B.J., 1993, "Computer Program for Calculation of Complex Chemical Equilibrium Compositions and Applications," Part I. Analysis. NASA RP-1311.
- Gracia-Salcedo, C.M., Brabbs, T.A., and McBride, B.J., 1988, "Experimental Verification of the Thermodynamic Properties for a Jet-A Fuel," NASA TM-101475.
- Gurvich, L.V. et al., 1978, *Thermodynamic Properties of Individual Substances*, Vol. 1, Pts. 1 & 2, Nauka, Moscow, U.S.S.R.
- Gurvich, L.V. et al., 1979, *Thermodynamic Properties of Individual Substances*, Vol. 2, Pts. 1 & 2, Nauka, Moscow, U.S.S.R.
- Gurvich, L.V. et al., 1982, *Thermodynamic Properties of Individual Substances*, Vol. 3, Pts. 1 & 2, Nauka, Moscow, U.S.S.R.
- Gurvich, L.V., Veyts, I.V., and Alcock, C.B., 1989, *Thermodynamic Properties of Individual Substances*, 4th ed., Vol. 1, Pts. 1 & 2, Hemisphere Publishing Corp., Washington, DC.
- Gurvich, L.V., Veyts, I.V., and Alcock, C.B., 1991, *Thermodynamic Properties of Individual Substances*, 4th ed., Vol. 2, Pts. 1 & 2, Hemisphere Publishing Corp., Washington, D.C.
- Haar, L., 1968, "Thermodynamic Properties of Ammonia as an Ideal Gas," *National Bureau of Standards, Journal of Research*, Vol. 72A, No. 2, pp. 207–216.
- Haar, L., Gallagher, J.S., and Kell, G.S., 1984, *NBS/NRC Steam Tables*, Hemisphere Publishing Corp., Washington, DC.
- Herzberg, G., 1970, "The Dissociation Energy of the Hydrogen Molecule," *Journal of Molecular Spectroscopy*, Vol. 33, pp. 147–168.
- Hildenbrand, D.L., and Murad, E., 1970, "Dissociation Energy of NaO(g) and the Heat of Atomization of Na₂O(g)," *Journal of Chemical Physics*, Vol. 53, No. 9, pp. 3403–3408.
- Hills, A.J., and Howard, C.J., 1984, "Rate Coefficient Temperature Dependence and Branching Ratio for the OH + ClO Reaction," *Journal of Chemical Physics*, Vol. 81, No. 10, pp. 4458–4465.
- Hippler, H., and Troe, J., 1990, "Thermodynamic Properties of Benzyl Radicals: Enthalpy of Formation From Toluene, Benzyl Iodide, and Dibenzyl Dissociation Equilibria," *Journal of Physical Chemistry*, Vol. 94, pp. 3803–3806.
- Hitchcock, A.P., and Laposa, J.D., 1975, "Vibrational Frequencies of Toluene-d₅," *Journal of Molecular Spectroscopy*, Vol. 54, pp. 223–230.
- Honig, A., Mandel, M., Stinch, M.L., and Townes, C.H., 1954, "Microwave Spectra of the Alkali Halides," *Physical Review*, Vol. 96, No. 3, pp. 629–642.
- Jacox, M.E., 1988, "Electronic Energy Levels of Small Polyatomic Transient Molecules," *Journal of Physical and Chemical Reference Data*, Vol. 17, No. 2, pp. 269–511.
- Kanamori, H., Seki, K., and Hirota, E., 1987, "Infrared Diode Laser Kinetic Spectroscopy of the CCH Radical v₃ Band," *Journal of Chemical Physics*, Vol. 87, No. 1, pp. 73–76.
- Kanamori, H., and Hirota, E., 1988, "Vibronic Bands of the CCH Radical Observed by Infrared Diode Laser Kinetic Spectroscopy," *Journal of Chemical Physics*, Vol. 89, No. 7, pp. 3962–3969.
- Keenan, J.H., Keyes, F.G., Hill, P.G., and Moore, J.G., 1969, *Steam Tables*. John Wiley & Sons, Inc., New York.
- Knoppers, W., VanHelvoort, K.V., Stolte, S., and Reuss, J., 1985, "Raman Overtone Spectroscopy of Ethylene," *Chemical Physics*, Vol. 98, pp. 1–6.
- Kudchadker, S.A., Kudchadker, A.P., Wilhoit, R.C., and Zwolinski, B.J., 1978, "Ideal Gas Thermodynamic Properties of Phenol and Cresols," *Journal of Physical and Chemical Reference Data*, Vol. 7, No. 2, p. 417–423.
- Lewis, G.N., Randall, M., Pitzer, K.S., and Brewer, L., 1961, *Thermodynamics*. McGraw-Hill, New York.
- Martin, W.C., and Zalubas, R., 1981, "Energy Levels of Sodium, Na I through Na XI," *Journal of Physical and Chemical Reference Data*, Vol. 10, No. 1, pp. 153–195.
- McBride, B.J., and Gordon, S., 1967, "FORTRAN IV Program for Calculation of Thermodynamic Data," NASA TN-4097.
- McBride, B.J., and Gordon, S., 1992, "Computer Program for Calculating and Fitting Thermodynamic Functions," NASA RP-1271.
- McBride, B.J., Gordon, S., and Reno, M.A., 1993, "Thermodynamic Data for Fifty Reference Elements," NASA TP-3287.
- Moore, C.B., and Pimentel, G.C., 1963, "Infrared Spectrum and Vibrational Potential Function of Ketene and the Deuterated Ketenes," *Journal of Chemical Physics*, Vol. 38, No. 12, pp. 2816–2829.
- Moore, C.E., 1970, "Selected Tables of Atomic Spectra," NSRDS-NBS 3, Sec. 3.
- Moore, C.E., 1971, "Atomic Energy Levels," Vols. 1, 2, and 3, NSRDS-NBS 35.
- Moore, C.E., 1972, "Selected Tables of Atomic Spectra," NSRDS-NBS 3, Sec. 6.
- Moore, C.E., 1975, "Selected Tables of Atomic Spectra," NSRDS-NBS 3, Sec. 5.
- Moore, C.E., 1976, "Selected Tables of Atomic Spectra," NSRDS-NBS 3, Sec. 7.
- Nagarajan, G., 1963, "Potential Constants and Thermodynamic Functions of the Tetrachlorides of Titanium and Vanadium," *Bulletin de la Societe Chimique Belgeum*, Vol. 72, pp. 346–350.
- Oetting, F.L., 1964, "Low-Temperature Heat Capacity and Related Thermodynamic Functions of Propylene Oxide." *Journal of Chemical Physics*, Vol. 41, No. 1, pp. 149–153.
- Osamura, Y., Schaefer, H.F., Gray, S.K., and Miller, W.H., 1981, "Vinylidene: A Very Shallow Minimum on the C₂H₂ Potential Energy Surface, Static and Dynamical Considerations," *Journal of the American Chemical Society*, Vol. 103, No. 8, pp. 1904–1907.

- Pamidimukkala, K.M., Rogers, D., and Skinner, G.B., 1982, "Ideal Gas Thermodynamic Properties of CH_3 , CD_3 , CD_4 , C_2D_2 , C_2D_4 , C_2D_6 , C_2H_6 , $\text{CH}_3\text{N}_2\text{CH}_3$, and $\text{CD}_3\text{N}_2\text{CD}_3$," *Journal of Physical and Chemical Standards, Journal of Research, Pt. A, Physics & Chemistry*, Vol. 73A, No. 5, pp. 493–498.
- Parker, V.B., Wagman, D.D., and Evans, W.H., 1971, "Selected Values of Chemical Thermodynamic Properties," NBS TN 270–6.
- Pedley, J.B., and Marshall, E.M., 1983, "Thermochemical Data for Gaseous Monoxides," *Journal of Physical and Chemical Reference Data*, Vol. 12, No. 4, pp. 967–1031.
- Pedley, J.B. Nylor, R.D., and Kirby, S.P., 1986, *Thermochemical Data of Organic Compounds*, Chapman & Hall, New York.
- Peric, M., Peyerimhoff, S.D., and Buenker, R.J., 1991, "Ab Initio Investigation of the Vibronic Structure in the C_2H Spectrum, III. Calculation of Vibronic Energies and Transition Probabilities in the $\text{X}^2\Sigma^+$, $\text{A}^2\Pi$ System," *Journal of Molecular Spectroscopy*, Vol. 148, pp. 180–200.
- Radhakrishnan, K., and Bittker, D.A., 1993, "LSENS, A General Chemical Kinetics and Sensitivity Analysis Code for Gas-Phase Reactions: User's Guide," NASA TM-105851.
- Rice, S.A., and Klemperer, W., 1957, "Spectra of the Alkali Halides, II. The Infrared Spectra of the Sodium and Potassium Halides, RbCl and CsCl ," *Journal of Chemical Physics*, Vol. 27, No. 2, pp. 573–579.
- Rodgers, A.S., Chao, J., Wilhoit, R.C., and Zwolinski, B.J., 1974, "Ideal Gas Thermodynamic Properties of Eight Chloro- and Fluoromethanes," *Journal of Physical and Chemical Reference Data*, Vol. 3, No. 1, pp. 117–140.
- Rudolph, H.D., Dreizler, H., Jaeschke, A., and Wendling, P., 1967, "Mikrowellenspektrum, Hinderungspotential der Internen Rotation und Dipolmoment des Toluols," *Zeitschrift fuer Naturforschung*, Vol. 22A, pp. 940–944.
- Seetula, J.A., and Gutman, D., 1992, Kinetics of the $\text{CH}_2\text{OH} + \text{HBr}$ and $\text{CH}_2\text{OH} + \text{HI}$ Reactions and Determination of the Heat of Formation of CH_2OH . *Journal of Physical Chemistry*, Vol. 96, pp. 5401–5405.
- Shimanouchi, T., 1972, "Tables of Molecular Vibrational Frequencies, Consolidated Vol. I," NSRDS-NBS 39.
- Shimanouchi, T., 1977, "Tables of Molecular Vibrational Frequencies, Consolidated Vol. II," *Journal of Physical and Chemical Reference Data*, Vol. 6, No. 3, pp. 993–1102.
- Spangenberg, H.J., Borger, I., and Schirmer, W., 1974, "Thermodynamic Functions of Various Hydrocarbon Nitrogen Compounds and Radicals at High-Temperatures and Composition of CHN-Plasmas," *Z. Phys. Chemie Leipzig*, Vol. 255, pp. 1–15.
- Stimson, H.F., 1969, "Some Precise Measurements of the Vapor Pressure of Water in the Range From 25 to 100 deg C," *National Bureau of Standards, Journal of Research, Pt. A, Physics & Chemistry*, Vol. 73A, No. 5, pp. 493–498.
- Sugar, J., and Corliss, C., 1979, "Energy Levels of Calcium, Ca I Through Ca XX," *Journal of Physical and Chemical Reference Data*, Vol. 8, No. 3, pp. 865–916.
- Svehla, R.A., 1962, "Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures," NASA TR R-132.
- Swalen, J.D., and Herschbach, D.R., 1957, "Internal Barrier of Propylene Oxide From the Microwave Spectrum," *Journal of Chemical Physics*, Vol. 27, No. 1, pp. 100–108.
- Trambarulo, R., and Gordy, W., 1950, "The Microwave Spectrum and Structure of Methyl Acetylene," *Journal of Chemical Physics*, Vol. 18, No. 12, pp. 1613–1616.
- TRC Thermodynamic Tables, Non-Hydrocarbons. TRC Thermodynamic Tables, Hydrocarbons.* Thermodynamics Research Center, Texas A&M University, College Station, TX, (loose-leaf tables with individual dates).
- Tsang, W., 1985, "The Stability of Alkyl Radicals," *Journal of the American Chemical Society*, Vol. 107, No. 10, pp. 2872–2880.
- Tsang, W., 1991, "Chemical Kinetic Data Base for Combustion Chemistry, Pt. V.: Propane," *Journal of Physical and Chemical Reference Data*, Vol. 20, No. 2, pp. 221–273.
- Villarreal, J.R., and Laane, J., 1975, "Raman Spectra and Internal Rotation of Methylcyclopropane and Its Analogs," *Journal of Chemical Physics*, Vol. 62, No. 1, pp. 303–304.
- Wagman, D.D., Evans, W.H., Parker, V.B., Schumm, R.H., Halow, I., Bailey, S.M., Churney, K.L., and Nuttall, R.L., 1982, "The NBS Tables of Chemical Thermodynamic Properties," *Journal of Physical and Chemical Reference Data*, Vol. 11, Supplement No. 2.
- Wagman, D.D., Evans, W.H., Parker, V.B., Halow, I., Bailey, S.M., Schumm, R.H., and Churney, K.L., 1971, "Selected Values of Chemical Thermodynamic Properties," NBS TN 270–5.
- Wicks, C.E., and Block, F.E., 1963, "Thermodynamic Properties of 65 Elements – Their Oxides, Halides, Carbides, and Nitrides," *Bureau of Mines Bulletin 605*.
- Wilhoit, R.C., 1975, *Thermodynamics Research Center Current Data News*, Vol. 3, No. 2.
- Woolley, H.W., 1987, "Ideal Gas Thermodynamic Functions for Water," *National Bureau of Standards, Journal of Research*, Vol. 92, No. 1, pp. 35–53.
- Zeleznik, F.J., and Gordon, S., 1961, "Simultaneous Least-Squares Approximations of a Function and Its First Integrals With Applications to Thermodynamic Data," NASA TN D-767.

TABLE I.—FORMAT FOR THERMODYNAMIC DATA COEFFICIENTS IN TABLE II

Record	Contents	Format	Columns
1	Species name Reference/date code Chemical formula: symbols and numbers “G” for gaseous species, “C” for condensed Temperature range Molecular weight Integer 1	A15 A6 4 (A2, F3.0) A1 2F10.3 F13.5 I1	1–15 19–24 25–44 45 46–65 66–78 80
2	Coefficients $a_i (i = 1,5)$ in eq. (1) for $T \geq 1000$ K	5E15.8	1–75
3	Integer 2 Coefficients b_1 and b_2 in eqs. (2) and (3) for $T \geq 1000$ K Coefficients $a_i (i = 1,3)$ in eq. (1) for $T \leq 1000$ K	I1 2E15.8 3E15.8 I1	80 1–30 31–75 80
4	Integer 3 Coefficients $a_i (i = 4,5)$ in eq. (1) for $T \leq 1000$ K Coefficients b_1 and b_2 in eqs. (2) and (3) for $T \leq 1000$ K $H^\circ (298.15)/R$, K Integer 4	2E15.8 2E15.8 E15.8 I1	1–30 31–60 61–75 80

Example:

BeOH J12/75BE 1.0 1.H 1. 0.G 300.000 5000.000 26.01952 1
 4.61167200E+00 2.39720130E-03-8.54891620E-07 1.43090620E-10-9.11123990E-15 2
 -1.53618380E+04-1.98829219E+00 1.91391480E+00 1.35071590E-02-1.85316870E-05 3
 1.29424710E-08-3.54389610E-12-1.48196830E+04 1.09928304E+01-1.37885210E+04 4



Empirical equations for this example

$$\text{Heat capacity : } \frac{C_p^\circ(T)}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (1)$$

$$\text{Enthalpy : } \frac{H^\circ(T)}{RT} = a_1 + a_2 \frac{T}{2} + a_3 \frac{T^2}{3} + a_4 \frac{T^3}{4} + a_5 \frac{T^4}{5} + \frac{b_1}{T} \quad (2)$$

$$\text{Entropy : } \frac{S^\circ(T)}{R} = a_1 \ln T + a_2 T + a_3 \frac{T^2}{2} + a_4 \frac{T^3}{3} + a_5 \frac{T^4}{4} + b_2 \quad (3)$$