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Bonnie J. McBride
and Sanford Gordon

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Bonnie J. McBride
Lewis Research Center
Cleveland, Ohio

Sanford Gordon
Sanford Gordon and Associates
Cleveland, Ohio

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

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Summary

A computer program is described which (1) calculates thermodynamic functions (heat capacity, enthalpy, entropy, and Gibbs energy) for several optional forms of the partition function, (2) fits these functions to empirical equations by means of a least-squares fit, and (3) calculates, as a function of temperature, heats of formation and equilibrium constants.

The program provides several methods for calculating ideal gas properties. For monatomic gases, three methods are given which differ in the technique used for truncating the partition function. For diatomic and polyatomic molecules, five methods are given which differ in the corrections to the rigid-rotator harmonic-oscillator approximation. A method for estimating thermodynamic functions for some species is also given.

Introduction

The computer program PAC1 (Properties and Coefficients), documented in reference 1, was initially made available to outside organizations in 1967. Since that time, PAC1 has been continuously revised, updated, and extended. Inasmuch as the program continues to be widely requested and used, this report is being published to provide documentation for the current version, referred to as PAC91.

The two principal purposes for initially preparing PAC1 are still valid today, namely, (1) to provide a means for generating theoretical thermodynamic functions from molecular constant data and (2) to provide a means of fitting these functions to empirical equations by using a least-squares fit. The coefficients obtained from the fit may then be used to generate a library of thermodynamic data in a uniform and easy-to-use format for use in other computer codes. Several large compilations of selected or calculated thermodynamic data currently exist. (See refs. 2 to 4 for some examples of early compilations and refs. 5 to 9 for some examples of more recent compilations.) Nevertheless, in spite of these compilations, there is a continuing need for additional calculations due to (1) discovery of new species, (2) revision of existing molecular constant data and structural parameters, (3) need for data at temperatures other than those already published, (4) availability of new or revised heats of formation, dissociation, or transition, and (5) revision of fundamental constants or atomic weights. Calculations may also be needed to compare the results of assuming various possible forms of the partition function. In addition, as mentioned previously, there is often a preference for thermodynamic data in functional rather than tabular form.

In order to carry out these needs, the PAC91 program has been prepared to perform any combination of the following: (1) calculate thermodynamic functions (heat capacity, enthalpy, entropy, and Gibbs energy) for any set of 1 to 202 temperatures, (2) obtain a least-squares fit of the first three of these functions (either individually, two at a time, or all three simultaneously) for up to eight temperature intervals, and (3) calculate, as a function of temperature, heats of formation and equilibrium constants from assigned reference elements. The number 202 for temperatures is somewhat arbitrary but was selected to accommodate a schedule of temperatures from 100 to 20 000 K at every 100 K, $T = 298.15$ K, and one additional temperature, if desired, such as $T = 273.16$ K.

The thermodynamic functions for ideal gases may be calculated from molecular constant data using one of several partition function variations provided by the program. For monatomic gases, (1) one of three partition function cutoff techniques may be selected and (2) unobserved but predicted electronic energy levels may be included by the program. For diatomic and polyatomic gases, (1) one of five partition functions may be selected which differ in the correction factors for nonrigid rotation, anharmonicity, and vibration-rotation interactions and (2) excited electronic states may be included.

Several new capabilities that were added to the program since the last publication include (1) the estimation of thermodynamic properties by a group additivity method, (2) the ability to calculate properties for species with internal rotors, and (3) a method for extrapolating data to high temperatures.

For the purpose of additional processing, (1) known thermodynamic functions for solids, liquids, or gases may be read in directly or (2) thermodynamic functions may be calculated from heat capacity equations.

Because of the variety of options provided and the resulting variety of input data required, an objective was to provide for a relatively simple procedure for reading input data. This was accomplished by means of a uniform input format.

At the time reference 1 was written (1967) input was read in by means of punched cards. While punched cards are no longer used, 80-column records are still retained for input.

The program and the equations used are described in detail. Examples of input and output are given for a variety of species.

Calculation of Ideal Gas Thermodynamic Functions

For gaseous species, the thermodynamic functions may be calculated from spectroscopic constants. A general discussion of methods of calculation is given in references such as 1 and 8. Many of the equations will be repeated here for convenience. The properties are expressed as functions of the internal partition function Q; that is,

$$\frac{C_p^o}{R} = T^2 \frac{d^2(\ln Q)}{dT^2} + 2T \frac{d(\ln Q)}{dT} + \frac{5}{2} \tag{1}$$

$$\frac{H_T^o - H_0^o}{RT} = T \frac{d(\ln Q)}{dT} + \frac{5}{2} \tag{2}$$

$$\frac{S_T^o}{R} = T \frac{d(\ln Q)}{dT} + \ln Q + \frac{3}{2} \ln M + \frac{5}{2} \ln T + S_c \tag{3}$$

$$-\frac{G_T^o - H_0^o}{RT} = \frac{S_T^o}{R} - \frac{H_T^o - H_0^o}{RT} = \ln Q + \frac{3}{2} \ln M + \frac{5}{2} \ln T + S_c - \frac{5}{2} \tag{4}$$

where

$$S_c = \frac{5}{2} + \ln \left[\left(\frac{2\pi m_\mu k T_1}{h^2} \right)^{3/2} \frac{kT_1}{p_o} \right] \tag{5}$$

S_c is the Sackur-Tetrode constant. ($T_1 = 1$ K. Other symbols are defined in appendix A.) When $p_o = 100\,000$ Pa (1 bar), $S_c = -1.151693$. When $p_o = 101\,325$ Pa (1 atm), $S_c = -1.164856$. Thus, values of S_T^o/R in units of bars will be higher than corresponding values in units of atm by 0.013163. The values for S_c and other fundamental constants are obtained from reference 10. The values of these constants are contained in BLOCK DATA of the program and are given in the section BLOCK DATA.

The internal partition function Q in equations (1) to (4) is given by

$$Q = \sum_{m=1}^{L} Q^m \tag{6}$$

where Q^m is the internal partition function for the m^{th} electronic state and L is the number of electronic states.

Internal Partition Functions for Monatomic Gases

For monatomic molecules, internal energy consists of electronic energy only. Equation (6) then becomes

$$Q = \sum_{m=1}^{L} Q_e^m = \sum_{m=1}^{L} (2J_m + 1) e^{-\epsilon_m/kT} = \sum_{m=1}^{L} g_m e^{-\epsilon_m/kT} \tag{7}$$

where Q_e^m, J_m, ϵ_m, and g_m are the electronic energy partition function, total angular momentum quantum number, electronic excitation energy, and statistical weight, respectively, for the m^{th} electronic state.

Cutoff methods.—An infinite number of bound states exist below the ionization limit for a hypothetical isolated atom ($L = \infty$ in eq. (7)). Inasmuch as the partition function diverges and approaches infinity as $L \to \infty$, the summation must be cut off. Reviews of various cutoff methods are given in a number of references such as 1, 8, 11, and 12. The following review essentially repeats that given in reference 1.

The cutoff methods may be considered to be of the following types:

(1) No dependence on temperature or pressure
(2) Dependence on temperature only
(3) Dependence on temperature and pressure (or density) and possibly degree of ionization

In the first of the three types, the summation may include various numbers of levels. For example, only the ground state is used in the Saha equation (see ref. 13) and only valence states are included in reference 8. The summation of equation (7) may be over a fixed and usually arbitrary number of levels (as, e.g., in ref. 14) or equation (7) may be summed through all observed levels (as in ref. 15, e.g.).

The second cutoff type is temperature dependent. The ionization potential is reduced by a quantity referred to as the ionization potential lowering, which in this case is a function of temperature only. The partition function is then permitted to include only those levels below the lowered ionization potential. In reference 16 it was suggested that the ionization potential be lowered by an amount equal to the temperature function kT. This suggested method was used in reference 4. Other temperature functions are summarized in reference 11.

The first two cutoff types are distinguished by the fact that they permit the partition function and related thermodynamic properties to be calculated as functions of temperature only. For the third type, it is not possible to calculate the partition function by specifying temperature only. One cutoff technique of this type relates the highest permitted principal quantum number n to the number of particles per unit volume (number density) such as suggested by Bethe (see discussion in ref. 11). Another technique uses the ionization potential lowering procedure previously described, but in this case the quantity by which the potential is lowered is a function of electron and ionized particle number densities. Several such quantities are summarized in reference 11.

This last technique involves mixtures of species and therefore precludes, for all practical purposes, the possibility of generating tables for individual species as a function of

temperature only. This is due to the fact that the cutoff criterion needed to calculate the partition function depends on mixture composition, while the calculation of mixture composition depends on the partition function. Thus, an iterative procedure is required where the partition function at a specified temperature may be changing from one iteration to the next. Consequently, since PAC91 calculates thermodynamic properties only for pure species, just the first two cutoff types are considered in this report.

Inclusion of predicted levels.—In addition to the divergence problem, there is the problem of whether to include observed energy levels only or to also include levels for predicted terms which, so far, have not been observed. From atomic theory, as presented in texts such as reference 17, predicted terms can be derived. Some of these terms are given in tables 10 and 11 in reference 17; in tables 5 to 20 in reference 18; and in reference 19. An examination of the tabulated observed terms in references 18 and 19 shows that many predicted terms are missing, especially for the higher quantum numbers.

It has been shown that various series of levels can be represented by formulas such as the Rydberg or the Rydberg-Ritz formulas (e.g., ref. 20). The constants in these formulas can be determined from known levels and used to extrapolate for the unobserved levels. However, the number of observed levels differ from species to species and, therefore, some judgment must be exercised in obtaining these constants. An alternate, but considerably simpler, technique for filling in unobserved levels, which gives essentially the same results for the partition function for many species as does the use of the Rydberg-Ritz equations, is included in the program. This alternate technique will now be described.

When the statistical weights g_i corresponding to predicted terms were examined, it was determined that for many chemical elements the sum of the statistical weights can be expressed by the following simple function of the principal quantum number n (except for the ground state n of most species):

$$\sum g_i = \sum \left(2J_i + 1\right) = bn^2 \qquad (8)$$

Equation (8) applies only to terms arising from excitation of the emission electron and does not account for other possible terms. A table in reference 1 contains, for the first 20 chemical elements, (1) the derived constants b to be used in equation (8) to obtain $\Sigma\, g_i$ for any n above the ground state and (2) $\Sigma\, g_i$ values for the ground state. In reference 12, this table was extended to include all the first 86 elements except for the lanthanide series (elements 58 through 71). Table 5 from reference 12 (p. 28) appears in this report as table I. The total quantum number above the ground state is given as a function of n in equation (8). However, in reference 12 it was recommended that, for some elements, the total quantum number above the ground state should be taken as a constant value (called c^*) for all values of n. Values of c^* are given in table I for elements 21 through 28, 39 through 46, 57, and 72 through 78.

The usefulness of equation (8) arises from the fact that the inclusion of an unobserved level generally makes considerably more difference in the partition function than does the error in the estimated energy for this level. Therefore, an option is provided in the PAC91 program to determine for each n the difference in statistical weight sums between the observed levels which have been read in as input and that given by equation (8). The program then adds this difference to the g_i of the highest observed level for the corresponding n.

This method of filling in predicted, but unobserved, levels by means of equation (8) was used to calculate the thermodynamic functions of the atomic species in reference 4.

Internal Partition Function for Diatomic and Polyatomic Molecules

Partition function.—For diatomic and polyatomic molecules, Q^m in equation (6) involves vibrational and rotational as well as electronic energy. In this report the following factored form is used to calculate Q^m:

$$Q^m = Q_e^m Q_V^m Q_R^m Q_\rho^m Q_\theta^m Q_W^m Q_c^m$$

or

$$\ln Q^m = \ln Q_e^m + \ln Q_V^m + \ln Q_R^m + \ln Q_\rho^m + \ln Q_\theta^m + \ln Q_W^m + \ln Q_c^m \qquad (9)$$

A recent review of formula details for these individual contributions to Q is given in reference 8. Some earlier references are as follows. The quantities Q_e^m, Q_V^m, and Q_R^m are the electronic, harmonic-oscillator, and classical-rotation contributions to the partition function, respectively, as given in standard texts (see refs. 21 to 24). The remaining quantities in equation (9) are the following correction factors: rotational stretching (centrifugal distortion) Q_ρ^m (refs. 24 to 26), low-temperature rigid rotation Q_θ^m (refs. 24 and 27), Fermi resonance Q_W^m (ref. 28), and both anharmonicity and vibration-rotation interaction Q_c^m (refs. 29 to 31).

The program provides five methods of calculating the partition function which vary in the inclusion of, and formulas for, the correction terms ($\ln Q_\rho^m$, $\ln Q_\theta^m$, $\ln Q_W^m$, and $\ln Q_c^m$). This provision is made so that the results of the various methods may be compared.

Table II contains detailed formulas for all the $\ln Q^m$ terms and their derivatives except those for $\ln Q_c^m$ which are given in table III. The derivatives of $\ln Q_c^m$ are not given directly as are the derivatives in table II. It was found to be considerably more convenient to express the derivatives of $\ln Q_c^m$ by means of general formulas than to obtain the derivatives directly. These general formulas are given in a footnote to table III.

Internal rotations.—A number of species, such as propylene oxide or hydrogen peroxide, have internal rotation. Energy levels for internal rotation may be calculated from potential functions, usually of the form

$$V = \frac{1}{2} \sum V_n(1 - \cos n\phi) \tag{10}$$

where V is the potential, V_n an n-fold barrier, n an integer from 1 to 6, and ϕ the phase angle. These energy levels may then be used to calculate the internal rotation contribution to the thermodynamic functions.

A computer program for calculating the energy levels and thermodynamic functions for the equation (10) potential was written by J. Laane and Associates based on the analysis in reference 32. This program was incorporated into PAC91 with necessary modifications. In addition, an option was added to calculate the contribution of a free rotor.

The subroutines which are involved in the hindered rotation calculation are INTROT, IROTOR, HMAT, EIGEN, and PRINT. A brief description of these routines is given in the section **Main Routines and Subroutines**.

Group Additivity Method

Several methods are available for estimating thermodynamic properties when molecular constant data for calculating partition functions are not available (e.g., see refs. 33 to 39). One of these methods is the group additivity method. S.W. Benson and coworkers have presented extensive tables of group properties for use with this method (refs. 35 and 36). These group properties permit estimating the heat of formation and entropy at 298.15 K and heat capacities from 300 to 1000 or 1500 K (depending on the group). In reference 37 Stein presents heat capacity properties to 3000 K for 18 groups pertaining to hydrocarbons.

Specialized techniques exist for obtaining estimates from group properties which may give more accuracy than that of Benson's method (e.g., refs. 38 and 39). However, Benson's method is accepted for PAC91 because of its relative simplicity, good accuracy, and application to a wide variety of species.

Empirical Equations For Thermodynamic Functions

Empirical equations for thermodynamic functions are often used for convenience. In dimensionless form, equations for heat capacity are usually of the following type:

$$\frac{C_p^o}{R} = \sum_{i=1}^{r} a_i T^{q_i} \tag{11}$$

where the exponent q_i may be zero or either a positive or negative whole or fractional number.

Enthalpy and entropy are related thermodynamically to C_R^o/R as follows:

$$\frac{H_T^o}{RT} = \frac{b_1}{T} + \frac{\int C_p^o\, dT}{RT} \tag{12}$$

$$\frac{S_T^o}{R} = b_2 + \int \left(\frac{C_p^o}{RT}\right) dT \tag{13}$$

where b_1 and b_2 are integration constants.

In equation (12) all terms are divided by T in order to make the equation dimensionless. The program uses equations (11) to (13) in two ways: (1) in generating the coefficients a_i and b_j from a set of thermodynamic data using the least-squares technique given in reference 40 or (2) conversely in generating the thermodynamic data from the empirical equations. Some details of the least-squares method are given in the section **Least-squares fit**.

Assigned Enthalpy Values

For some applications (see ref. 41) it is convenient to combine sensible enthalpy 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 the various substances, inasmuch as only differences in enthalpy are measurable. For example, the arbitrary base selected in reference 4 was a value of zero at 298.15 K ($H_{298.15}^o = 0$) for a selected set of elements. This base was also selected for PAC91. It makes the assigned value, $H_{298.15}^o$, of any substance equal to its heat of formation at 298.15 K from this set of selected elements.

Assigned Reference Elements

The designation of an element in a particular phase to be a reference element is needed in order that values of heats of formation $\Delta_f H_T^o$ and equilibrium constants $\log_{10} K$ be unambiguously related to specific reactions. Reference 42 gives thermodynamic functions, phases, transition temperatures, and heats of transition for the following 50 elements plus deuterium and election gas: Ag, Al, Ar, B, Ba, Be, Br_2, C, Ca, Cd, Cl_2, Co, Cr, Cs, Cu, D_2, e^-, F_2, Fe, Ge, H_2, He, Hg, I_2, K, Kr, Li, Mg, Mn, Mo, N_2, Na, Nb, Ne, Ni, O_2, P, Pb, Rb, S, Si, Sn, Sr, Ta, Th, Ti, U, V, W, Xe, Zn, and Zr. The enthalpy and free energy values from reference 42 have been stored on a file (referred to herein as the EF data file) for the purpose of $\Delta_f H_T^o$ and $\log_{10} K$ calculations.

Heats of Formation and Equilibrium Constants

In the program described in this report, heats of formation and $\log_{10}K$ for a species are calculated as functions of temperature for the formation of the species from the elements in their assigned reference state. The following is an example of how these properties are calculated for CO(g) at 1000 K:

$$\Delta_f H^o_{1000} = \left(H^o_{1000}\right)_{CO(g)} - \left(H^o_{1000}\right)_{C(graphite)} - \frac{1}{2}\left(H^o_{1000}\right)_{O_2(g)} \tag{14}$$

$$\Delta_f G^o_{1000} = \left(G^o_{1000}\right)_{CO(g)} - \left(G^o_{1000}\right)_{C(graphite)} - \frac{1}{2}\left(G^o_{1000}\right)_{O_2(g)} \tag{15}$$

By definition,

$$\log_{10}K = \frac{-\Delta_f G^o_T}{2.3025851\ RT} \tag{16}$$

Computer Program

The computer program PAC91 was written in ANSI standard Fortran 77. PAC91 should work on any system with sufficient storage. There are about 5500 lines in the source code which uses about 300 kilobytes of memory. The compiled program takes about 390 kilobytes.

Some input and output files are stored in the standard I/O units 5 and 6, respectively. Other I/O units are used in conjunction with least-squares coefficients, EF data sets, and group additivity data (see section "Saved Output" in appendix C). These nonstandard I/O units are as follows:

I/O unit	Contents or function
10	Least-squares coefficients
11	Formatted EF data
13	Unformatted EF data
14	Scratch unit for formatted EF data
17	Scratch unit for unformatted EF data
19	Group additivity data

No OPEN statements for the I/O units were included in the source program.

Availability to Other Organizations

The PAC91 program can be obtained for a fee from COSMIC (Computer Software Management Information Center) at the following address:

COSMIC
382 East Broad Street
Athens, GA 30602
Tel: (404) 542-3265
FAX: (404) 542-4807

The program will generally be sent out on a diskette which contains the following four files:

File number	Contents
1	PAC91 source program
2	EF data sets for reference elements
3	Least-squares coefficients for additivity groups
4	Input data sets for examples

The preparation of files 2 and 3 is discussed in the section "Saved output" in appendix C. File 4 contains the input for the eight examples given in appendix D which can serve as test cases for checking out the program. Files 2, 3, and 4 require approximately 160, 24, and 10.2 kilobytes, respectively.

Input Data Codes

The input for a particular species is a set of 80-column records. There are many alphanumeric code words in these records. These code words use capital letters and numbers and have a maximum length of six characters. They either (1) indicate an option; (2) identify a record; or (3) describe the information that follows it.

These code words will be used throughout the report. The input code words in columns 1 to 6 will be referred to as record IDs. Elsewhere on the record, they will be referred to as labels. An index of code words is given in table XI which may be helpful in locating definitions, discussions, and examples. A complete discussion of input format is given in appendix B.

Options

The program provides a choice of several methods for calculating the thermodynamic functions C^o_p, $H^o_T - H^o_0$, $H^o_T - H^o_{298.15}$, S^o_T, $-(G^o_T - H^o_0)$, and $-(G^o_T - H^o_{298.15})$. For ideal gases, these functions may be obtained from one of several assumed forms of the partition function, from empirical equations, or, for some hydrocarbons, from the group additivity method. For solids and liquids, the thermodynamic functions may be calculated only from empirical equations. In addition, thermodynamic functions for any phase of a species may be read in directly for additional processing.

The program also has two other capabilities which are optional: (1) least-squares fitting of the thermodynamic functions to empirical equations (eqs. (11) to (13)) and (2) calculating heats of formation and $\log_{10}K$ values for the same temperature range as the functions.

The following is a discussion of these optional features.

Partition functions—monatomic gases.—The partition function for monatomic gases is given by equation (7). The program permits three optional ways of terminating the number of energy levels L to be included in calculating this partition function. These three options, indicated by their input code names, are: (1) ALLN—inclusion of all electronic levels in the input data, (2) FIXEDN—inclusion of all levels through a specified principal quantum number n, and (3) TEMPER—inclusion of all energy levels that are less than or equal to the ionization potential lowered by an amount kT (see section **Cutoff methods**).

With any of these three cutoff options, an additional option (FILL) is provided to include predicted but unobserved levels automatically (see discussion in the section **Inclusion of predicted levels**). All of these options are labels on the METHOD record (see table VI).

Partition functions—diatomic and polyatomic gases.—For diatomic and polyatomic gases, the program provides for a selection of five methods of calculating the partition function. These methods vary in the inclusion of, and formulas for, the correction terms ($\ln Q_\rho$, $\ln Q_\theta$, $\ln Q_W$, and $\ln Q_c$) in equation (9). The formulas for the $\ln Q$ terms included in each of the five methods are given in tables II and III. If certain spectroscopic constants are not available as input, the program automatically excludes those $\ln Q$ terms involving them. The methods (with their METHOD record labels given in parentheses) are as follows:

(1) Rigid-Rotator Harmonic-Oscillator (RRHO) approximation—This method excludes all the correction terms in equation (9) (i.e., $\ln Q_\rho$, $\ln Q_\theta$, $\ln Q_W$, and $\ln Q_c$).

(2) Modified Pennington and Kobe (PANDK) method—The formulas given in table III for $\ln Q_c$ are similar to those given in reference 29. The method in this report is equivalent to the one described in reference 4 except for the formula for $\ln Q_\theta$ (formula 6 in table II). All correction terms in equation (9) are included with the exception of the Fermi resonance $\ln Q_W$ as indicated in table II.

(3) Joint Army Navy Air Force (JANAF) method—This method is described and used in reference 6. For diatomic molecules, it is the same as the PANDK method except for the definitions of a_1 and X_{11} which are used in formulas 9 and 12, respectively, in table III. For polyatomic molecules, the JANAF method is the same as the RRHO method.

(4) Nonrigid-Rotator Anharmonic-Oscillator 1 (NRRAO1)—In addition to the $\ln Q_\theta$ and $\ln Q_\rho$ terms, all the $\ln Q_c$ terms given in references 30 and 31 were included which do not contain a $(c_2/T)^2$ or $(c_2/T)^3$ factor.

(5) Nonrigid-Rotator Anharmonic-Oscillator 2 (NRRAO2)—This method includes the same $\ln Q_c$ terms as NRRAO1 with the addition of $\ln Q_c$ terms from references 30 and 31 which contain $(c_2/T)^2$ factors.

METHOD record labels are summarized in table VI.

Internal rotation contributions.—As described in the section **Internal rotations**, PAC91 includes the capability of calculating the contributions of internal rotation, free or hindered. The contribution of each internal rotor replaces the contribution of a fundamental frequency. Thus the total number of fundamental frequencies (including degeneracies) plus the number of internal rotors remains $3N$–6, where N is the number of atoms in the molecule.

Estimation by group additivity method.—As mentioned previously, PAC91 provides an option for estimating thermodynamic properties by a group additivity method. At present, thermodynamic properties for just 34 groups have been prepared for use with PAC91 (see section **Input**). These group properties permit estimating properties for some but not all hydrocarbons (e.g., groups for cyclic and fused hydrocarbons are not included). The group properties are in the form of least-squares coefficients with C_p^o represented as a fourth-order polynomial. The additivity method requires identifying the various groups comprising the species. This is discussed further in the sections **Input** and **Data records for ADD method** in appendix B and in example 2 in appendix D).

Thermodynamic functions from empirical equations.—The routine for calculating thermodynamic functions from the empirical equations (eqs. (11) to (13)) has the following features:

(1) The value of r (number of coefficients a_i) may be any number from 1 to 8.

(2) The temperature exponents q_i may be zero or any positive or negative whole or fractional number.

(3) Any number of sets of a_i and q_i may be read in for various temperature intervals for a particular species.

(4) The integration constants b_1 and b_2 may be read in or calculated by the program from the enthalpy and entropy values, respectively, for a specific temperature.

(5) When a phase transition occurs, the integration constants b_1 and b_2 for the second phase may be read in or calculated by the program from either the enthalpy or entropy of transition.

(6) There is an option to write the heat capacity coefficients and the two integration constants for each temperature interval on I/O unit 10.

Least-squares fit.—The least-squares routine fits the thermodynamic functions C_p^o/R, H_T^o/RT, and S_T^o/R to equations (11), (12), and (13) either individually, any two simultaneously, or all three simultaneously (the default option). The selection of the appropriate labels for fitting any one function or any two simultaneously is discussed in the section **LSTSQS record(s)** in appendix B. The least-squares fit has the following additional features:

(1) The value of r (number of coefficients a_i) may be any number from 1 to 8. (In PAC1, r was 1 to 10.)

(2) The temperature exponents q_i may be zero or any positive or negative whole or fractional number.

(3) An option is provided to permit the data to be divided into any number of specified intervals from 1 to 8. The purpose in providing for several intervals is to increase the accuracy of the fit. (In PAC1, the number of intervals was 1 to 9.)

(4) The equations for each temperature interval are usually

constrained at an endpoint to fit either the original data or the values obtained from fitting an adjacent interval. However, there is an option to remove the constraint by use of the label NOCNS. The purpose of these constraints is to give equal values of the functions at the common point and thus avoid discontinuities between consecutive intervals. Also, only one temperature may be specified in the input for which the fitted equations reproduce the original values. (If no temperature is specified, the program assigns 298.15 K. In PAC1 the default assigned temperature was 1000 K.)

(5) For two or more phases, if an enthalpy of transition (labeled DELTAH) or an entropy of transition (labeled DELTAS) is given, the original data as well as the least-squares fitted data will be constrained so that $T\Delta_{tr}S^o_T = \Delta_{tr}H^o_T$.

(6) For each temperature interval, the coefficients a_i for heat capacity plus the two integration constants will be written on I/O unit 10. (In PAC1, these data were punched on binary cards.)

(7) If the temperature exponents q_i (EXP labels on the LSTSQS records) are not specified, PAC91 defaults to the following form of equation (11):

$$\frac{C^o_p}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4 \tag{17}$$

and corresponding forms for H^o_T/RT and S^o_T/R (see table VIII).

(8) The equations for C^o_p/R may be the same or different for each temperature interval.

(9) At least as many values of C^o_p (or C^o_p/R) are required as the number of exponents in equation (11) or equation (17). If fewer C^o_p (or C^o_p/R) values are given in the input than the number of exponents requested, PAC91 automatically reduces the number of exponents to the number of C^o_p or C^o_p/R values.

It should be noted that the present format for the least-squares coefficients differs from that of PAC1. Details of the present format are given in table VIII.

Extrapolation by Wilhoit's method.—Occasionally data are given in the literature to only relatively low temperatures (say to 1000 or 1500 K) but data may be needed to higher temperatures for some applications (such as shock tube data analysis). As has been pointed out (see ref. 5), extrapolation of thermodynamic data with the functional form described in the previous section may give bad results. An example is the extrapolation of data for iso-octane which are given in reference 7 to 1500 K. The least-squares coefficients which are generated from these data give an extrapolated value at 3000 K of $C^o_p/R = -3331$. This impossible situation can be avoided by obtaining extrapolated values from a method for fitting data presented by Wilhoit (ref. 43). Wilhoit gives the following equation for C^o_p:

$$C^o_p = C^o_p(0) + \left[C^o_p(\infty) - C^o_p(0)\right]y^2\left[1 + (y-1)\sum_{i=0}^{n} a_iy^i\right] \tag{18}$$

where $y = T/(T + S)$ (y varying from 0 to 1), S a scaling factor, $C^o_p(0)$ the low temperature limit for C^o_p, $C^o_p(\infty)$ the high temperature limit for C^o_p, and a_i the least-squares coefficients. $C^o_p(0)$ includes only rotational and translational contributions ($C^o_p(0) = 3.5R$ for linear and $4R$ for nonlinear species) while $C^o_p(\infty)$ also includes the vibrational contributions. The total contributions result in $C^o_p(\infty) = (3N - 1.5)R$ for linear and $(3N - 2)R$ for nonlinear species, where N is the number of atoms in the molecule.

A computer program for this method with $n = 3$ in equation (18) is given in appendix B of reference 5. This program was somewhat modified and incorporated into PAC91 as subroutines WILHOI and WCALC. While the original Wilhoit method is presented in reference 43 as a method of fitting data rather than extrapolating data, PAC91 uses these subroutines only for the purpose of extrapolation. The general procedure involved in PAC91 in using these subroutines is

(1) The original input data are fitted to Wilhoit's functional form and the Wilhoit coefficients are generated.

(2) These coefficients are then used to extrapolate the thermodynamic data to various specified temperatures.

(3) The original data and the extrapolated data are then refit to the PAC91 functional form.

For the example of iso-octane mentioned previously, the use of the Wilhoit fit for extrapolation gives a reasonable value of $C^o_p/R = 75.299$ at 3000 K. (The classical value is $C^o_p(\infty)/R = 76.$) Additional examples using Wilhoit extrapolation are given for examples 2 and 3 in appendix D.

In addition to the usual input data, the use of the Wilhoit method for extrapolation requires a WILH label on a METHOD record. The program also requires knowledge with this method of whether the species is linear or nonlinear. Unless specified otherwise, the program assumes the species is nonlinear. For linear species, the label LINE is required.

Heat of formation and $\log_{10}K$ values.—The program provides an option for calculating, as a function of temperature, heats of formation and $\log_{10}K$ values of a species formed from its reference elements (see sections **Assigned Reference Elements** and **Heats of Formation and Equilibrium Constants**). These values for a particular species can be calculated if the necessary enthalpy and free energy data for the reference elements (referred to as EF data) are available. Therefore, the assigned reference elements are processed first. For these reference elements there is an option to save the enthalpy and free energy data in two ways: (1) in an unformatted form on I/O unit 13 replacing any data for the element already in the library and (2) in a formatted form appending the data on I/O unit 11. (See appendix C for additional information on the contents of EF data saved on

I/O unit 11.) The data on I/O unit 13 are ready for immediate use. For backup purposes, the data on I/O unit 11 may be transferred to and included in a file containing EF data in formatted and readable form for all reference elements which have already been processed. These files replace the set of punched binary EF data cards of reference 1.

The data on I/O unit 13 are saved for use with other species being processed during the same computer run as well as for later computer runs. The data in the formatted EF data file discussed previously may be read in as part of the input and, if so, are automatically put on I/O unit 13. The newly read-in data replace data already on I/O unit 13 for any matching elements.

If there is a temperature in the data for a particular species which is not contained in the EF data for the required reference elements, the reference elements data are interpolated using three-point Lagrangian interpolation.

Output tables.—There are many options for listed output tables indicated on an OUTPUT record. The tables vary in the following ways: in whether they are original data or calculated from least-squares coefficients; in energy units (dimensionless, joules, or calories); and in whether the functions are given to many figures or are rounded and include columns for $\Delta_f H_T^o$ and $\log_{10} K$.

Input

Input data sets for any number of species may be combined into one file. The data in each set are read, processed, and cleared before the next set is read. A set of data for a diatomic gas, for example, would contain the chemical formula; the output options; the method of calculation, such as PANDK; molecular data such as ω_e, $\omega_e x_e$, B_e, and α_e; desired options such as a least-squares fit or a special temperature schedule; and, finally, the record ID FINISH to indicate the end of the set of data.

In addition to these input data sets, data contained in two general files are required for certain applications. The first of these two files contains enthalpy and free energy data (EF data) for reference elements which are used to calculate equilibrium constants $\log_{10} K$ and heats of formation $\Delta_f H_T^o$ (see section **Heat of formation and $\log_{10} K$ values**). An example of the contents of the EF data file for the element Mg is given in appendix D, example 6. The second general file contains thermodynamic data (in the form of least-squares coefficients) for various groups that are used to estimate properties of species (see section **Group Additivity Method**). These coefficients for 34 groups are given in table X and have the same format as that described in table VIII but these use a fourth-order polynomial for C_p^o.

The references from which most of the data were taken to generate these coefficients are given in table IX. In addition, table IX gives the labels used in PAC91 for these groups, Benson's notation (ref. 36), the group structure, and the atoms contained in the group. Of the 34 groups given, thermodynamic data for 18 were taken from reference 36 and 12 from reference 37. Thermodynamic properties for the remaining 4 groups were calculated by the PAC91 program using data from the following references:

Species		References	
Formula	Name	$\Delta_f H_{298.15}^o$	Spectroscopic constants
C_2H_2	Acetylene	7	8
C_2H	Ethynyl radical	44	45
C_2H_4	Ethylene	7	46,47
C_2H_3	Vinyl radical	44	8
C_2H_3	Stabilized vinyl radical	[a]44,48	[b]8
C_6H_6	Benzene	7	49
C_6H_5	Phenyl radical	7	49

[a]$\Delta_f H_{298.15}^o$ is taken to be the same as that for the vinyl radical plus an estimated resonance stabilization energy of 8 kcal/mole taken from reference 48.
[b]Assumed to be the same as for the vinyl radical.

Uniform format.—Many types of input are used in PAC91. To facilitate the preparation of this input, a uniform format was devised for the original version of this program (ref. 1) for most input data. This format is retained for the present program as well. While in the original version, input was read in from 80 column punched cards, in the present program input is in the form of 80 column records. Details of the uniform format are given in appendix B.

Contents of individual records.—A brief description of the contents of the individual records is given in table IV. (Detailed descriptions are given in appendix B.) The right-hand column indicates which records are optional. The word in columns 1 to 6 on all records except the formula record will be referred to as the record ID. Words in other columns will generally be referred to as labels. While the record ID may contain up to six characters the PAC91 program will use only the first four characters of the code to identify the record. The code is intended to be a mnemonic device. Thus, for example, the LSTSQS record contains information for the least-squares fit of the thermodynamic data. Since the program uses only the first four characters, the word LSTS is required for this record, while characters in columns 5 and 6 are optional.

As shown in table IV, the record ID does one or more of the following:

(1) Indicates what information is in the record (e.g., NAME, REFN, OUTPUT, TEMP, LSTSQS, or CTEM).

(2) Identifies the data on the records which follow it (e.g., METHOD and EFDA).

(3) Calls for some intermediate output (i.e., LISTEF).

(4) Indicates the end of a set of data (i.e., FINISH).

General Flow of Program

(1) Each record (except for the EF data) is read and listed. The flow is directed according to the record ID.

(2) The input data (including options) are cleared at the beginning of the program and after each FINISH record ID.

(3) There may be any number of sets of data—each having any combination of options and each ending with a FINISH code.

(4) The records NAME, formula, LSTSQS, OUTPUT, DATE, and REFNCE should come ahead of the METHOD record but their order is immaterial.

(5) Any record ID ahead of the METHOD record ID which is not recognized by PAC91 will be assumed to be a chemical formula record.

(6) From the chemical formula, the following items are determined by the program:

(a) molecular weight

(b) phase of the species

(c) number of atoms (i.e., whether species is monatomic, diatomic, or polyatomic)

(7) The H_0^o value may be calculated from an assigned enthalpy value at any temperature or a heat of formation (see chemical formula record in appendix B and table V). (The H_0^o value is used in calculating $\Delta_f H_T^o$ and $\log_{10} K$ and the integration constant b_1 (eq. (12)).

(8) The temperature schedule (TEMP record), if not the standard 100(100)6000 K, must be read before each METHOD record giving the calculation method. However, it should be noted that TEMP records are not used with method READIN inasmuch as temperatures for the READIN method are given on the data records.

(9) The data records must follow the METHOD record.

(10) Thermodynamic functions are calculated immediately after PAC91 reads a record ID different from the one it was reading in the data records.

(11) After the FINISH code is read, a check is made for the LSQS and LOGK options from the OUTPUT record. Also, tables of thermodynamic functions are listed (from original data and, if the CTAB label is on the OUTPUT record, from least-squares coefficients).

(12) With an EFTAPE label on an OUTPUT record for a reference element, the EF data for that element will be written on I/O units 11 and 13. The data on I/O unit 13 will be available for use with any succeeding calculations.

(13) Any number of sets of METHOD record and corresponding data records may be read for a set of input data. This is useful for species with more than one phase in the temperature range of interest. For example, the thermodynamic functions for the solid may be read in directly while the liquid data may be obtained from empirical equations. The data for both phases will appear in the same listed tables of the thermodynamic properties.

(14) Contributions of excited electronic states may be included in the calculation of the thermodynamic functions for diatomic and polyatomic gases. There may be any number of states, each having its own set of molecular constants. This is accomplished by grouping the data records for each state together with a code number in columns 79 and 80. The values of Q^m, $T\,dQ^m/dT$, and $T^2\,d^2Q^m/dT^2$ are calculated after the data records for each state are read. These values are summed as they are calculated.

Output

Most of the output are tables of thermodynamic data. These data may be *original* data calculated by PAC91 according to one of the methods specified by a METHOD record or the data may be calculated from least-squares coefficients generated by PAC91 with the LSQS option. Original data tables have the word ORIGINAL on the first line of the table and on the last line of each page. Tables with data from least-squares coefficients have the word COEFFICIENTS on the first line of the table and on the last line of each page.

Other possible types of output include input data, the least-squares errors table, EF data, and intermediate output. A brief description of output data is given in this section. Additional details are given in appendix C.

Input data.—The contents of all input records in the uniform format are always listed in the output. Some additional information calculated by PAC91 such as molecular weight and Wilhoit parameters are interspersed with the record images.

Tables of thermodynamic properties.—There may be ten possible tables of functions printed for the temperature schedules. The tables vary according to the labels on the OUTPUT records. Five are for *original* data. With a CTAB label, a corresponding five possibilities are for thermodynamic functions calculated from the least-squares coefficients. With the MFIG label, three of the five possible tables are given to many figures (usually from 6 or 7 to 10 or 11). With the LOGK label, the remaining two tables are rounded to the same number of figures as in the JANAF tables (ref. 6) and also may contain values of $\Delta_f H_T^o$ and $\log_{10} K$. The three many-figured tables and the two rounded tables vary in the energy units which must be specified with label options. The JOULES label is required for energy units in joules and the CAL label for energy units in calories. Only the many-figured tables have an option for dimensionless units (label DMLESS). The temperature schedule for the *original* data is either the default schedule, temperatures read in with data, or a schedule set by the TEMP records. The coefficients data will have the same schedule unless a special schedule is given with CTEM records.

Table of least-squares errors.—These tables are listed with the LSQS option. They provide information concerning the accuracy of the fit. The word "error" in the output refers to the difference between the original and fitted data. In addition to listing the least-squares coefficients for each temperature interval, the following information is listed: (1) the thermodynamic functions (both the original and those obtained from the least-squares fit for each temperature, (2) the errors between the original and the fitted data for each temperature, and (3) average, maximum, and least-squares errors and relative errors for C_p^o/R, $(H_T^o - H_0^o)/RT$, S_T^o/R, and $-(G_T^o - H_0^o)/RT$.

Intermediate output.—With an INTERM label on the OUTPUT record, additional intermediate data are listed as detailed in appendix C. These intermediate data are often useful for debugging purposes.

EF data.—EF data for a reference element contain the enthalpy and Gibbs energy data for that reference element. These data are required for $\log_{10}K$ and $\Delta_f H_T^o$ calculations for compounds containing that element. See sections **Listed Output** and **Saved Output** in appendix C for additional discussion of EF data.

Examples

Eight sample problems were selected to illustrate a number of the methods and options of PAC91. The input data files, listed output and some discussion of these examples are given in appendix D.

Main Routine and Subroutines

The previous program (PAC1) consists of a main routine and 17 subroutines. The present program (PAC91) consists of a main routine, 24 subroutines, and BLOCK DATA. One function, KD, was dropped from the previous program and eight new subroutines and BLOCK DATA were added. Of these eight new subroutines, five are for internal rotation (EIGEN, HMAT, INTROT, IROTOR, and PRINT); two are for extrapolation by the Wilhoit method (WCALC and WILHOI); and one is for the group additivity method (GROUP). The remaining 16 subroutines from PAC1 were extensively revised to accommodate more modern computers.

A short description of each subroutine follows.

ATOM.—This routine calculates thermodynamic functions for monatomic gases.

The routine calls INPUT to read all data records plus the next record. The J_i or g_i values (eq. (7)), which are read with an alphanumeric format, are changed to floating point numbers and stored.

Energy levels are sorted in order of increasing energy values. The number of levels included in the calculations is determined by the cutoff method (ALLN, FIXEDN, or TEMPER) given on the METHOD record. Predicted but unobserved levels will be included with the FILL option.

DELH.—This routine has several functions. It calculates the H_0^o value from information given on the formula card (either heat of formation at 298.15 K (HF298), heat of formation at any temperature ($\Delta_f H_T^o$) and the corresponding temperature T, or an assigned enthalpy H_T^o and the corresponding temperature T). If a LSQS label has been included on the OUTPUT record, subroutine LEAST is called to perform a least-squares fit. Subroutine PUNCH is called to write least-squares coefficients on I/O units 6 and 10. The coefficients may also have been read in with method COEF if a TCOEF label is included on the data records.

Subroutine DELH is called from the main program after the FINISH card has been read. However, it will also be called from RECO for phase transition points. In this latter case, any processing (the H_0^o calculation, the least-squares fit, or the writing of coefficients) will be for the species phase coming ahead of the transition point in the input. For example, for a species with input data for the solid followed by the liquid, DELH will process the solid when it has been called from RECO. The liquid will be processed when DELH is called from the main program.

DERIV.—This subroutine calculates the first and second derivatives of the logarithm of Q_c^m (the anharmonicity and vibration-rotation interaction contribution to the total partition function Q^m). It uses the special method given in footnote e of table III. The routine is called from a number of places in LINK1. The values of the variables in the call vector of DERIV are calculated in LINK1.

EFTAPE and entry EFLIST.—Subroutine EFTAPE and entry EFLIST are concerned with preparing, reading, and writing the enthalpy and free energy data records of reference elements (EF data). These EF data are used in conjunction with the option of calculating tables of $\log_{10}K$ and $\Delta_f H_T^o$ for any species. Subroutine EFTAPE is called under two circumstances: (1) if an EFTAPE label is included on an OUTPUT record of a reference element and (2) if an EFDA record is read. Entry EFLIST is called when a LISTEF record is read.

In the first case of subroutine EFTAPE being called (by an EFTAPE label on the OUTPUT record), the formatted EF data set for the reference element being processed is written on I/O units 6 and 11 and the unformatted data set is written on I/O unit 13.

An EF data set for the reference element currently being processed may already exist on I/O unit 13 from a previous run or from being read in from a special file (see section **Saved output**). In this event, the EF data set for the current run replaces the existing EF data set for this reference element on I/O unit 13. Otherwise, the current EF data set is written at the end of all other EF data sets on I/O unit 13.

In the second case (EFDA record is read), subroutine EFTAPE is called to read data created in the first case and previously written on I/O unit 11. These data are usually backup data or data that come with the program. The subroutine merges the data with the unformatted form of the data on I/O unit 13.

Entry EFLIST writes the contents of I/O unit 13 into I/O unit 6 in order to obtain a legible listing of the EF data for all reference elements currently in the I/O unit 13 file.

EIGEN.—This is one of the five subroutines associated with the calculation of the contribution of internal rotation to thermodynamic functions. It is called by HMAT and solves for the eigenvalues of the Hamiltonian matrix which are then used to obtain the energy levels of the rotor(s).

GROUP.—Subroutine GROUP is called from the Main Program when the label ADD is included on the METHOD record. Subroutine GROUP locates and adds together the contributions of various groups specified in the input. The group contributions are in the form of least-squares coefficients

(see table X) and, when added together, produce the least-squares coefficients for the desired species. Occasionally, for a special configuration such as gauche, a constant correction is required for H_T°/R. For this case, the correction may be included in the input with the label HRCO.

HMAT.—This is one of the five subroutines associated with the calculation of the contribution of internal rotation to thermodynamic functions. It calculates the elements HINT (I,J) for a Hamiltonian matrix. It is called by IROTOR. HMAT, in turn, calls EIGEN to solve the matrix for the energy levels of the rotor.

IDENT.—This routine analyzes the chemical formula on either the formula record or the EFDA record. It separates and stores each chemical symbol and corresponding number of atoms in the chemical formula. The chemical symbols are matched with the SYMBOL array stored from BLOCK DATA. Corresponding indexes are stored. When analyzing a chemical formula from a formula record the molecular weight is calculated.

INPUT.—This routine is called from the main program. It reads and lists all standard input from I/O unit 5 except the thermodynamic data following the EFDA record and unformatted data. I/O unit 14 is used as a scratch unit for reading in data.

INTROT.—This is one of the five subroutines involved with internal rotation. It calculates the contribution of the internal rotor(s) to the partition function and its first and second derivatives. It uses the energy levels which are generated in subroutines HMAT and EIGEN. It is called from LINK1.

IROTOR.—This is one of the five subroutines involved with internal rotation. It is called from POLY if the label INTROT appears in the input data set. IROTOR calls INPUT to obtain the necessary input for internal rotation calculations (hindered or free). The potential function is then calculated and stored for optional printout (see subroutine PRINT). IROTOR then calls HMAT to set up a Hamiltonian matrix which is then solved in EIGEN to obtain the energy levels for the rotor. For each rotor present, IROTOR then calculates the relative value of the energy levels of the rotor above the lowest energy for that rotor. A maximum of four unique rotors is permitted.

LEAST.—This routine is called from DELH only if the LSQS label was included on the OUTPUT record. It calculates the least-squares coefficients and lists certain information comparing original thermodynamic functions with those calculated from the coefficients. See **Tables of least-squares errors** and **Least-squares coefficients** in appendix C.

LINK1.—This routine calculates the partition function for diatomic and polyatomic gases. The formulas given in tables II and III are evaluated according to the method specified.

The routine is called from subroutine POLY. LINK1 in turn calls two subroutines, DERIV to calculate the derivatives of the partition function and QSUM to keep a running total of the various contributions to the partition function.

LOGK.—This routine is called from the main program only if a LOGK label has been included on the OUTPUT record. It calculates $\Delta_f H_T^\circ/RT$, $\Delta_f H_T^\circ$, $-\Delta_f G_T^\circ/RT$, and $\log_{10} K$ for the formation of the species from the assigned reference elements. The required enthalpy and free-energy data for these reference elements have been previously stored in the file on I/O unit 13 by the EFTAPE subroutine.

The LOGK routine lists the two tables of rounded properties as detailed in appendix C. If any required data for the reference elements of the species being processed are not on I/O unit 13, the appropriate columns in these two tables are left blank.

PAGEID.—This routine is called from a number of places and lists three items of information at the bottom of a page in the output listing and skips to a new page. The three items are (1) the name in columns 7–22 on the NAME records; (2) the word COEFFICIENTS if the page contains thermodynamic properties from least-squares coefficients or ORIGINAL if otherwise; and (3) either BAR or ATM to designate the standard reference unit of pressure as being either one bar or one atmosphere. PAGEID allows approximately 55 lines to be printed on a page. Up to six names from NAME records are saved and printed.

POLY.—This routine calculates thermodynamic functions for diatomic and polyatomic gases. It is called from the main program.

Subroutine INPUT is called from POLY to read the data records plus the next record. Subroutine LINK1 is called to calculate the partition function according to the method specified (RRHO, PANDK, JANAF, NRRAO1, or NRRAO2).

If more than one electronic state is present, the various states are identified by a code in columns 79 to 80 of the data records. In this case, data records for only one state at a time are read in and stored. The partition function for each state is calculated prior to processing data records for the next state.

PRINT.—This is one of five subroutines involved with internal rotation. This subroutine prints the number of energy levels and values of the potential function specified by NOUT (a label in a data record). It is called from IROTOR as an option only if NOUT is greater than zero.

PUNCH.—This routine writes on I/O units 6 and 10 the coefficients obtained either from a least-squares fit or from the data records associated with method COEF. PUNCH is called from subroutine DELH. See output details in appendix C.

QSUM.—This routine keeps a running total of all, except translational, contributions to the partition function and its derivative for each electronic state. These contributions are listed if an INTERM label has been included on the OUTPUT record. QSUM is called from a number of places in LINK1.

RECO.—The routine is called from the main program after reading a METHOD record which contains either a COEF or READIN label. The RECO routine calls INPUT to read the data records plus the next record.

For READIN, the temperature and the thermodynamic functions on each record are simply stored. For COEF, the thermodynamic functions are calculated for the temperatures on the temperature schedule and stored.

The RECO routine is also used to relate the enthalpy of two phases of the same species by means of an enthalpy or entropy of transition. One of these transition values is given on the

METHOD record of the second phase (DELTAH or DELTAS labels, see table VI) and used to calculate the enthalpy of the second phase at the transition temperature. The Gibbs energy value of the second phase is taken to be equal to the Gibbs energy value of the first phase at the transition temperature.

If a transition is present, the routine calls DELH (discussed in the section "DELH") to check for the options of least-squares fit or storing coefficients for the first phase.

TABLES.—This routine is called from the main program for printing the many-figured tables (MFIG on the OUTPUT record). It lists tables of thermodynamic functions for three sets of energy units for either *original* or *coefficients* data as discussed in appendix C. The format varies depending on the availability of the following values: (1) the $H^o_{298.15} - H^o_0$ value which is required in obtaining $H^o_T - H^o_{298.15}$ and $-(G^o_T - H^o_{298.15})$, and (2) the H^o_0 value which is required in obtaining H^o_T and $-G^o_T$.

TEMPER.—This routine stores the temperature schedules as given on TEMP or CTEM records. The TEMP records are for *original* data and CTEM for *coefficients* data. The routine is called from the main program after a TEMP record has been read and just before the *coefficients* tables are processed.

WCALC.—This is one of the two subroutines pertaining to the Wilhoit method of fitting thermodynamic data. It is called by subroutine WILHOI to calculate thermodynamic functions from Wilhoit coefficients.

WILHOI.—This is one of the two subroutines pertaining to the Wilhoit method of fitting thermodynamic data. It is used in PAC91 only for the purpose of extrapolation. WILHOI is called in the main program if the label WILH has been included on a METHOD record. It generates the Wilhoit coefficients used in WCALC to extrapolate data. The desired temperature schedule for extrapolation is specified with TEMP input records.

BLOCK DATA.—BLOCK DATA contains the fundamental constants and information concerning chemical elements from hydrogen (atomic number 1) through californium (atomic number 98) and also electron gas and deuterium. These data consist of the following information for each element:

(1) Chemical symbol
(2) Atomic weight
(3) Constant b in equation (8) or c^* for FILL option (see section **Inclusion of predicted levels**, and table I)
(4) Sum of statistical weights for ground state (for FILL option)
(5) Phase
(6) Atomic number
(7) Number of atoms in most abundant form of the element at room temperature

The atomic weights were taken from reference 50. The fundamental constants were taken from reference 10. The Sackur-Tetrode constant is given in equation (5). Other constants are as follows:

$$R = 8.31451 \text{ kJ/kg-mol-K}$$

$$c_2 = (hc/k) = 1.438769 \text{ cm-K}$$

Appendix A—Symbols

A_e, B_e, C_e	rotational constants corresponding to equilibrium separation of atoms
A_0, B_0, C_0	rotational constants for lowest vibrational state
a_i	temperature coefficients in eq. (11)
b	constant defined in eq. (8)
b_1	integration constant defined by eq. (12)
b_2	integration constant defined by eq. (13)
C_p^o	heat capacity at constant pressure for standard state
$C_p^o(0)$	heat capacity at constant pressure at 0 K
$C_p^o(\infty)$	heat capacity at constant pressure at infinite temperature
c	velocity of light
cr	crystal phase of chemical substance
c_2	second radiation constant, hc/k
c^*	constant representing total quantum weight for each principal quantum number n above ground state n for some elements (see table I)
D_e	spectroscopic constants for rotational stretching
D_0, D_{000}	rotational stretching constants for lowest vibrational state
d_i	degeneracy associated with ν_i
G_T^o	either $(G_T^o - H_0^o) + H_0^o$ or $(G_T^o - H_{298.15}^o) + H_{298.15}^o$
$G_T^o - H_0^o$	Gibbs energy at temperature T relative to enthalpy at 0 K for standard state
$G_T^o - H_{298.15}^o$	Gibbs energy at temperature T relative to enthalpy at 298.15 K for standard state
$\Delta_f G_T^o$	Gibbs energy of formation of a substance at temperature T from its reference elements in their standard state
g_i, g_m	electronic statistical weight
g_{ii}	anharmonicity constant for doubly degenerate vibrations in linear molecules
H_0^o	chemical energy at 0 K for standard state
$H_{298.15}^o$	assigned enthalpy at 298.15 K for standard state (equal to $\Delta_f H_{298.15}^o$)
H_T^o	either $(H_T^o - H_0^o) + H_0^o$ or $(H_T^o - H_{298.15}^o) + H_{298.15}^o$
$H_T^o - H_0^o$	sensible enthalpy at temperature T relative to 0 K for standard state
$H_T^o - H_{298.15}^o$	sensible enthalpy at temperature T relative to 298.15 K for standard state
$\Delta_f H_T^o$	enthalpy of formation (heat of formation) of a substance at temperature T from its reference elements in their standard state
$\Delta_{trs} H_T^o$	enthalpy of transition between two phases of a substance at temperature T
$\Delta_{trs} S_T^o$	entropy of transition between two phases of a substance at temperature T
h	Planck constant
I_A, I_B, I_C	principal moments of inertia
J_i, J_m	total angular momentum quantum number
K	equilibrium constant
k	Boltzmann constant
L	total number of electronic energy states
ℓ	liquid phase of chemical substance
M	molecular weight
m_μ	atomic mass constant
N	number of atoms in molecule
n	number of unique frequencies, number of phase angles, or principal quantum number
p_o	standard state pressure in eq. (5)
Q	internal partition function
Q^m	internal partition function for m^{th} electronic state
Q_c^m	correction factor to the partition function for anharmonicity and vibration-rotation interaction for m^{th} electronic state
Q_e^m	electronic partition function for m^{th} electronic state
Q_R^m	classical rotation partition function for m^{th} electronic state
Q_V^m	harmonic-oscillator partition function for m^{th} electronic state
Q_W^m	Fermi resonance correction factor to partition function for m^{th} electronic state
Q_θ^m	low temperature rigid rotational correction factor to partition function for m^{th} electronic state
Q_ρ^m	rotational-stretching—correction factor to partition function for m^{th} electronic state
q_i	temperature exponents in eq. (11)
R	universal gas constant
r	number of coefficients a_i in eq. (11)
S_c	constant defined by eq. (5)
S_T^o	entropy at temperature T for standard state

T	temperature, K
T_0	electronic excitation energy between lowest vibrational states ($v = 0$) of ground and excited state for diatomic and polyatomic gases
T_1	temperature, 1 K
u_i	$c_2\nu_i/T$
V	potential
V_n	n-fold barrier
v,v_i	vibrational quantum number
W_0	Fermi resonance constant
x_{ij},y_{ijk}	anharmonicity constants for polyatomic molecules
α_e,α_i	vibration-rotation interaction constants for diatomic and linear polyatomic molecules
α_i^A,α_i^B,α_i^C,α_{ij}	vibration-rotation interaction constants for polyatomic molecules
β_i	rotational-stretching—vibration interaction constant
ϵ_m	energy of m^{th} electronic state
ν_i	observed fundamental frequency
ρ	rotational-stretching spectroscopic constant
σ	symmetry number
ω_e	zero-order vibrational frequency for diatomic molecule
$\omega_e x_e$,$\omega_e y_e$,$\omega_e z_e$	anharmonicity constants for diatomic molecules

Appendix B—Details in Preparing Input

Uniform Format

With a few exceptions, all input records are read in with an 80-column uniform format, namely A6, 4(A6, D12.0), I2. The exceptions are the formula, NAME and REFNCE records discussed in the section **Description of Input Records**. Another exception is EF data; however, EF data records are prepared by the program and not the user (see section **EFDA and EF data records**). The record columns for the uniform format are as follows:

	Record ID	Label 1	Numerical value 1	Label 2	Numerical value 2	Label 3	Numerical value 3	Label 4	Numerical value 4	
Record columns	1-6	7-12	13-24	25-30	31-42	43-48	49-60	61-66	67-78	79-80
Format	A6	A6	D12.0	A6	D12.0	A6	D12.0	A6	D12.0	I2

The labels (label 1, label 2, . . .) are codes on all types of input records except one. (The exception, described in the section **Data records for the FIXEDN, ALLN, or TEMPER methods**, is the record containing spectroscopic data for atoms.) These codes serve two purposes. One purpose is to specify an option in the program. For example, the label RRHO specifies a method of calculation. The second purpose is to identify the number which follows it. For example, the label STATWT precedes the numerical value of the statistical weight.

The last two columns (79 and 80) are used for several purposes:

(1) For atomic gases, the principal quantum numbers are put in these columns, right- adjusted, for methods FIXEDN and TEMPER. (See example 1 in appendix D.)

(2) For diatomic and polyatomic gases, the electronic level identification is put in these columns if excited states are included.

(3) For polyatomic gases with molecular data and internal rotors, the integers in these columns indicate the rotor to which the data belong.

(4) On the LSTSQS record, if different equations are used for different temperature intervals, the integer in column 80 indicates the interval associated with the information on the remainder of the record. Integers range from 1 to 8, with 1 assigned to the lowest temperature interval. (See example 1 in appendix D.)

Some general rules in preparing the input are as follows:

(1) With one exception, record ID's (columns 1 to 6) and labels are alphanumeric and must be left-adjusted. The exception is that the labels on the data records which contain spectroscopic constants for monatomic gases are numbers and do not need to be left-adjusted. (See section **Data records** in this appendix and example 1 in appendix D.)

(2) All blank labels are ignored by the program.

(3) Each numerical value must be immediately preceded by its label. However, the order of values is usually immaterial. Exceptions are noted in the details for the individual records.

(4) The numerical values may be the following:

(a) A right-adjusted integer

(b) A floating-point number without exponent (e.g., 0.00021), anywhere in the field

(c) A right-adjusted floating-point number with exponent indicating decimal place (e.g., 2.1-4 is 2.1×10^{-4})

(5) The last two columns (79 and 80) are right-adjusted integers.

Order of Input Records

Some discussion on the order of the input records is given in the section **General Flow of the Program**. Specific instructions for placement of the individual records are given in the details for preparing the records.

For a single computer run, there may be any number of species processed where each species requires its own set of input data. The set of input data records for each species should generally be in the following order:

(1) NAME record. While this record is optional, it is usually convenient to be first. Part of the contents of this record appears with least-squares coefficients output and also on the bottom of output listings. When there are multiple phases (indicated by two temperatures in the temperature schedule being adjacent and equal), there should be a corresponding NAME record for each phase. See example 8 in appendix D.

(2) Formula record (must be the first nonoptional record in the set)

(3) Miscellaneous records in any order containing options and information (namely, DATE, REFNCE, OUTPUT or CTEM)

(4) TEMP record(s), if any
(5) METHOD record
(6) Data record(s)
(7) FINISH record

} There may be more than one set of these records for a single species. (See examples 6 and 8, appendix D.)

There are two kinds of input records not directly related to input data sets, namely the LISTEF record and the EF data records.

Description of Input Records

Examples of the individual records discussed in this section are given in appendix D. All input records except the formula record are identified by a record ID (columns 1 to 6). However, PAC91 reads only the first four of the first six columns of the record ID. Six columns were reserved in order to provide a little more assistance in identifying the record. For example, the term METHOD is more descriptive than METH. However, either METH in columns 1 to 4 or METHOD in columns 1 to 6 is equally acceptable.

CTEM record.—The purpose of these records is to provide a temperature schedule for output tables generated from least-squares coefficients. However, the tables from coefficients will be printed only if the label CTAB is on the OUTPUT record. If no CTEM records are included in the input data set, the program will default to the temperature schedule of the original data. The labels associated with CTEM (T and I) and their corresponding numerical values have the same definitions as those used with the TEMP record. (See **TEMP record.**)

Data records.—These records follow the METHOD record and contain the input data required by the method. Except for the spectroscopic data of monatomic gases (see example 1, appendix D), the labels are codes identifying the numerical values that follow them. Table VII is a summary of the labels and numerical values to be used on data records for the various methods given in table VI. The data records may optionally contain identifying information in columns 1 to 6. For example, in the sample problems of appendix D, the species C_4H_4 (example 3) has the identifying word C4H4 in columns 1 to 6 of its data records. By contrast, columns 1 to 6 are blank for the species Na_2CO_3(s) (example 8). However, whatever appears in columns 1 to 6 on the first data record, blank or otherwise, must also appear in columns 1 to 6 on all the remaining data records in the input data set. No data records are associated with METHOD WILH. A further description of the data records for various methods follows:

Data records for the READIN *method*: Generally, each record contains four labels with the four corresponding numerical values as indicated in table VII. The four labels correspond to temperature, heat capacity, enthalpy, and either entropy or Gibbs energy. Temperature, which must always be given, has the label T; however, for the other three properties there are several options of labels as given in table VII depending on the data to which they correspond. If enthalpy and Gibbs energy are referred to $H^o_{298.15}$ rather than H^o_0, the $H^o_{298.15} - H^o_0$ value must be included on the METHOD record (label H298H0) if $H^o_T - H^o_0$ values are desired in the final tables. (See examples 6 and 8, appendix D.)

Sometimes one or two of the three properties are omitted in the data records or ignored by the PAC91 program. This occurs when there are LSTSQS records that include one or two of the NOCP, NOH, or NOS labels. See **LSTSQS records.**

Data records for the COEF *method*: The coefficient and exponent values for each set of empirical equations (eqs. (11) to (13)) must be preceded by the values of the temperature limits (T labels in table VII) for which the equation applies (see examples 6 and 8, appendix D). The lower T value must be the first numerical value.

Occasionally the coefficients a_i $(i = 1, r)$ are available while the integration constants for enthalpy and entropy b_1 and b_2 are not. For this case, b_1 and b_2 values may be calculated by the program in one of the following ways:

(1) Reading in an enthalpy and an entropy or Gibbs energy value with the corresponding temperature on the first record. The labels and values should be the same as for the data records for the READIN method except that C^o_p or C^o_p/R may be omitted.

(2) Using the value of enthalpy or entropy of transition (DELTAH or DELTAS on the METHOD record (see table VI)). This method may be used only when the two phases related by the transition value are being processed in the same run. The reason is that the transition value is combined with the enthalpy or entropy value for the last temperature of the preceding phase. (See examples 6 and 8, appendix D.)

With the COEF method the TCOEF label provides an option to write these coefficients on I/O unit 10 in the same format as least-squares coefficients. (See table VIII.) For each set of coefficients, the temperature intervals may be specified in two different ways:

(1) If only the TCOEF label is given with no additional information on the record concerning temperature intervals, the temperature intervals will be taken from the T values accompanying the coefficient data (see Mg(ℓ), example 6, and $Na_2CO_3(\ell)$, example 8, appendix D).

(2) Any temperature intervals may be specified by TCOEF labels and corresponding values which give the endpoints of the intervals. These values may or may not be the same as the T values for the set.

Data records for the FIXEDN, ALLN, *or* TEMPER *methods*: In contrast to all other types of records using the uniform format, these records use the label columns as well as the numerical columns for numbers. The labels contain either the total angular momentum quantum number J_m or the electronic statistical weight g_m (eq. (7)), and the numerical values contain the excitation energy ϵ_m/hc (eq. (7)) in centimeters^{-1}. If g_m values are used, the label GLABEL must be included on the METHOD record. For either the FILL option or the FIXEDN method, the principal quantum numbers must be included in columns 79 to 80, right-adjusted. The data on the remaining portion of the record must correspond to that principal quantum number. (See example 1, appendix D, for the TEMPER method and FILL option.)

Data records for the RRHO, PANDK, JANAF, NRRAO1, *or* NRRAO2 *methods*: The equations for the partition function

of the various methods are given in tables I and II. The input data must always contain at least the following quantities for each electronic state:

(1) The fundamental vibrational frequencies of the molecule (ω_e or ν_i)
(2) Either the rotational constant(s) (B_0 for linear; A_0, B_0, and C_0 for nonlinear molecules) or the moment(s) of inertia (I_B for linear; I_A, I_B, and I_C for nonlinear molecules)
(3) The symmetry number
(4) The statistical weight

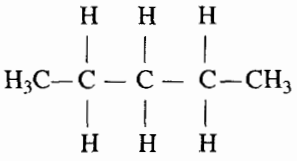
Other spectroscopic constants such as anharmonicity or rotation-vibration interaction constants are optional. If these optional constants are not included, correction terms involving them are automatically excluded from the partition function. (See example 4 (RRHO), example 7 (JANAF), and example 5 (NRRAO2) in appendix D.)

When excited electronic states are involved, the data for each state are read and processed separately. Therefore, the data records must be grouped together with an identifying number in columns 79 to 80. For example, the data for the 15 electronic states included in example 7, appendix D, are distinguished by the integers 1 to 15 in columns 79 and 80.

Data records for the ADD *method*: The label and quantity for each of the appropriate groups forming the desired species must appear on these records. Example 2 in appendix D illustrates the ADD method. Table IX facilitates the preparation of the records inasmuch as it contains the PAC91 label notation, the Benson notation, the structure, the elements contained in the group, and the references for the selected thermodynamic data. The following two examples, for n-pentane and i-pentane (2-methyl butane), are given to further illustrate the use of this method:

(1) n-pentane

(a) Structure:



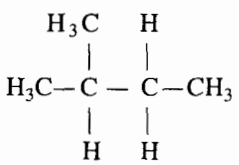
(b) Groups: $2CH_3$ and $3CH_2$

(c) Benson notation: $2C\text{-}(H)_3(C) + 3C\text{-}(H)_2(C)_2$

(d) PAC91 record: (label number label number)
CH3C 2. CH2C2 3.

(2) i-pentane

(a) Structure:



(b) Groups: $3CH_3$, $1CH_2$, and 1CH

(c) Benson notation: $3C\text{-}(H)_3(C) + C\text{-}(H)_2(C)_2 + C\text{-}(H)(C)_3$

(d) PAC91 record:
(label number label number label number)
CH3C 3. CH2C2 1. CHC3 1.
HRCO 402.6

The label HRCO on the second record is a correction term for the heat of formation due to the gauche interaction in i-pentane. Its value is obtained by dividing the value of 0.8 kcal/mole given in reference 36 by R = 1.987216 cal/mol-K. Other terms used in the ADD method are given in table VII.

DATE record.—The purpose of the DATE record is to include a date and/or reference code with the least-squares coefficient output. The record should contain only one label which will be included in the second record of the least-squares coefficient output for each species. (See examples 1 to 4 and 6 to 8, appendix D.)

EFDA and EF data records.—The data on these records are used in conjunction with the LOGK option to obtain $\log_{10}K$ and $\Delta_f H^o_T$ values. These records are prepared automatically by the program when an EFTAPE label is included on the OUTPUT record of a reference element. For each reference element which has been processed in this manner one EFDA record and a varying number of EF data records are prepared depending on the amount of thermodynamic data available for each reference element. The combination of the one EFDA record and EF data records which follow it will be referred to as EF data. The contents of an EFDA record consists of the chemical formula of the EF data reference element, the date code, the H^o_0/R value, the melting point, if any, and the number of temperatures for which there are enthalpy and Gibbs energy values following the EFDA record. Each EF data record consists of a temperature (K), an enthalpy $(H^o_T - H^o_0)/RT$ value, and a Gibbs energy $-(G^o_T - H^o_0)/RT$ value followed by a second temperature, enthalpy, and Gibbs energy. A listing of typical EF data for an element is shown in the output for Mg(s,ℓ), example 6, appendix D.

Additional discussion of EF data sets is given in the section **Saved Output** in appendix C.

FINISH record.—This required record is the last record in the input set for each species. It contains only the code FINISH in columns 1 to 6.

Formula record.—This is the first nonoptional record in the input data set for each species and is reserved for two pieces of information. First, the species formula, as detailed below, is always required. Second, either an assigned enthalpy or a heat of reaction value with the corresponding units and temperature is required only if the assigned enthalpy column (H^o_T or H^o_T/R) is desired in the output tables, or when calling

for either of the following two options:

(1) $\text{Log}_{10}K$ and $\Delta_f H^o_T$ calculations (also requires a LOGK label on an OUTPUT record), or

(2) Least-squares fit of the thermodynamic functions (also requires a LSQS label on an OUTPUT record)

All the examples in appendix D, with the exception of C_2H_3 (example 2), have either an assigned enthalpy ASINDH or a heat of formation HF298. C_2H_3 uses METHOD ADD which calculates the heat of formation.

The first 12 columns are reserved for the formula of the species. The formula should be left-adjusted and contain no blanks. It should be prepared in the following order:

(1) Each atomic symbol followed by the number of atoms even if the number is 1; these atomic symbols should all be in capital letters and correspond to the symbols in BLOCK DATA.

(2) For ionic species, the proper number of pluses or minuses

(3) For condensed species, a left parenthesis

(4) For condensed species other than reference elements, any character except G (e.g., an L for a liquid, an S for solid, or C for crystal)

(5) For condensed species to be used as reference elements, the character must be S for solid or L for liquid (in order to match the formula in BLOCK DATA).

(6) For condensed species, a right parenthesis

The following are some examples, primarily for ionized species:

Species	Columns 1 to 12
$CaCO_3(s)$	CA1C1O3(S)
F^-	F1−
N^+	N1+
O^{++}	O1++
O_2^-	O2−

The remainder of the record is reserved for a heat of formation, the energy units, and the temperature of the reaction. There are three forms in which the heat of formation may be expressed and six choices of units. These are summarized in table V.

LISTEF record.—This option is used to obtain a listing of the EF data stored on I/O unit 13.

LSTSQS record.—No least-squares calculations will be made without a LSQS label on the OUTPUT record. By contrast, the LSTSQS record is required only for specifying any of the nonstandard (or non-default) options pertaining to the least-squares fit of the functions C^o_p/R, H^o_T/RT, and S^o_T/R to equations (11) through (13). The options are summarized in table IV.

With a LSQS label and no LSTSQS record, the program will attempt the default options. They include the following:

(1) Fitting the three functions simultaneously

(2) Setting the q_i values in equation (11) to be −2, −1, 0, 1, 2, 3, and 4

(3) Setting two temperature intervals, 200 to 1000 and 1000 to 6000 K

(4) Constraining the fit to fit the three functions exactly at 298.15 K

(5) Constraining the fitted functions to match at 1000 K (The coefficients for the higher temperature interval are constrained to reproduce the fitted results of the lower temperature interval at 1000 K.)

If an OLD label is listed on the LSTSQS record, the default q_i values in equation (11) change to 0, 1, 2, 3, and 4, to match the *old* polynomial form used for C^o_p in reference 41.

If a NOCNS label is given, the fit is not constrained to fit any values of the functions. The fit may be constrained to fit the functions exactly at a specified temperature provided the temperature is in the temperature schedule of the data. This temperature value follows a TCONST label. In this case any common points between any succeeding intervals will be constrained to match.

The temperature intervals may be changed by using T labels, each followed by one value (namely, the first temperature, the breakpoints, and the final temperature, all in kelvin). The program will order these values from the lowest to the highest. Allowance is made for up to 8 intervals (9 values).

The q_i values in equation (11) may be set with EXP labels. These exponent values may be positive, negative, zero, or fractional. As always, the integers following a label must include a decimal point. The program orders these values from the lowest to the highest. The limit on the number of exponents (r in eq.(11)) is 8. Different sets of EXP values may be used for different temperature intervals by giving the appropriate temperature interval number in column 80 (with 1 referring to the lowest interval). If a set of EXP values is given without specifying an interval (i.e., column 80 is blank), this set will be used for all unspecified intervals. If there is no EXP set given with column 80 blank, the default set will be used for the unspecified intervals.

For fitting one function only or some combination of two functions the labels NOCP (no C^o_p), NOH (no H^o_T), and NOS (no S^o_T), are provided. The labels are used as follows:

Functions to be fit simultaneously	Label on LSTSQS record
C^o_p/R only	NOH and NOS
H^o_T/RT only	NOCP and NOS
S^o_T/R only	NOCP and NOH
C^o_p/R and H^o_T/RT	NOS
C^o_p/R and S^o_T/R	NOH
H^o_T/RT and S^o_T/R	NOCP

With NOS and NOH combinations, an enthalpy value is required to obtain the b_1 integration constant and an entropy value is required to obtain the b_2 constant. In this case, a TPROP label with its corresponding temperature is required on the record. PAC91 then expects to find the required

properties at this temperature in the data obtained from the METHOD and data records. When NOCP, NOH, or NOS labels are used, it is assumed these data (C_p^o, H_T^o, or S_T^o) for the remaining temperatures are either missing or wrong. PAC91 will fill these data with the values it gets from the least-squares fit, even for the *original* tables. These simultaneous fit combinations may vary between temperature intervals using the same method described above for the functional form. The temperature interval number is put in column 80 on the LSTSQS records with the appropriate parameters.

METHOD record.—This record follows the option records and must be included for any calculations to take place. It specifies the technique for obtaining the thermodynamic functions (see section **Options**) and immediately precedes the data required by the method (data records). The record has the code word METHOD in columns 1 to 6. The possible codes in the label and numerical value columns are summarized in table VI. The functions may be (1) calculated from molecular constants for ideal gases (labels FIXEDN, ALLN, or TEMPER for monatomic molecules and labels RRHO, PANDK, JANAF, NRRAO1, or NRRAO2 for diatomic and polyatomic molecules) (see examples 1, 4, 5, and 7, appendix D); (2) calculated from coefficients and exponents using equations (11) to (13) (label COEF), (see examples 6 and 8, appendix D); (3) read in directly (label READIN) (see examples 3, 6, and 8, appendix D); (4) estimated by a group addivity method (label ADD) (see example 2, appendix D); or (5) extrapolated functions using the Wilhoit method (label WILH, see examples 2 and 3, appendix D). The calculation techniques listed in (1) are discussed in the section **Calculation of Ideal Gas Thermodynamic Functions**.

In conjunction with these method labels, the METHOD record may contain some additional labels and information as indicated in table VI.

Occasionally, a single method may not apply to the entire desired temperature range for a species. In this case the following records must be included for each temperature interval, in order: (1) TEMP record(s) for the desired temperature interval (if the method is not READIN), (2) a METHOD record for this temperature interval, and (3) the associated data records. The sets should be in order of increasing temperature. (See examples 2, 3, 6 and 8, appendix D.)

The WILH method always follows another method and requires no data records to follow it. This method generates Wilhoit-fit coefficients in order to extrapolate thermodynamic data obtained from the previous method to higher temperatures. The temperature schedule for the extrapolation must be specified with TEMP records immediately preceding the WILH method record. If the species is linear, the label LINE must be specified (otherwise the default is to nonlinear).

NAME record.—This record contains a name and comments. PAC91 allows for up to six NAME records in a data set for a species. For least-squares coefficients, one name and associated comments are transferred to the output for each set of coefficients. Columns 7-24 are used for the name and columns 25-80 are used for comments (see table VIII).

Multiple NAME records are useful in identifying multiple phase or lambda transitions for condensed species. When PAC91 encounters the same temperature in two adjacent slots in the temperature schedule, it assumes there will be a new set of coefficients using the name and comments from the next NAME record, if there is one. If there is not, it uses the name and comments from the previous NAME record (see examples 6 and 8, appendix D).

OUTPUT record.—The OUTPUT records contain options for output. There are 10 possible labels for this purpose and no numerical values. These labels (options) are now summarized:

ATM label. Calls for pressure to be in units of atmospheres in the entropy and Gibbs energy values appearing in the output tables. The default units are bars.

CAL label. Calls for tables with calories as the energy units. The label must be combined with either MFIG or LOGK or both.

CTAB label. Calls for tables of functions calculated from coefficients to be printed. The label must be combined with either MFIG or LOGK or both.

DMLESS label. Calls for many-figured tables in dimensionless units.

EFTAPE label. Used with an assigned reference element whose data are needed for $\Delta_f H_T^o$ and $\log_{10} K$ calculations. Inclusion of the label causes the H_0^o value and the $(H_T^o - H_0^o)/RT$ and $-(G_T^o - H_0^o)/RT$ data for this species to be merged with the EF data on I/O unit 13 in unformatted form. These functions are also written on I/O unit 11 in formatted form. See example 6, appendix D.

INTERM label. Calls for intermediate output to be printed when thermodynamic functions are being calculated from molecular constants. (See section **Intermediate data with INTERM label**, appendix C and example 5, appendix D.)

JOULES label. Calls for tables with joules as the energy units. The label must be combined with MFIG or LOGK or both.

LOGK label. Causes rounded tables of thermodynamic properties including $\Delta_f H_T^o$ and $\log_{10} K$ to be listed. If no units label is specified, JOULES will be assumed. If the appropriate EF data are not available on I/O unit 13, the $\Delta_f H_T^o$ and $\log_{10} K$ columns will be left blank. If there is no matching temperature in the assigned reference element data, the data that are there will be interpolated by three-point Lagrangian interpolation. (See example 8, appendix D.)

LSQS label. Calls for a least-squares fit of the functions to equations (11) to (13). Unless otherwise specified on the LSTSQS record, the q_i values assigned will be -2, -1, 0, 1, 2, 3, and 4. If no T's are given, the temperature intervals assigned will be 200 to 1000 K and 1000 to 6000 K. For condensed species, transition points are automatically inserted.

MFIG label. Causes many-figured (unrounded) tables of functions to be printed. If no energy unit label is given, JOULES will be assumed.

REFNCE record.—The only purpose of this record is for comments such as identifying sources of input data. All the information in columns 7-80 in this record is alphanumeric. The usual labels and numerical values are ignored. (See examples 1, 3, 4, and 6, appendix D.)

TEMP record.—These records give a temperature schedule for which thermodynamic functions are to be calculated. The program allows for a maximum of 202 temperatures per species.

Each temperature in the desired temperature schedule may be specified individually with a T label. (See table IV.) However, if there are several temperatures incremented by a fixed amount, this part of the temperature schedule may be specified by giving, in order, the lowest temperature labeled T, the increment labeled I, and the highest temperature labeled T. For example, the temperature schedule, 100, 200, 298.15, 300, 400, 500, 600, 688.2, 700, 750, 800, 850, 900, 962.3, and 1000, could be designated as follows:

Record ID	Label 1	Numerical value 1	Label 2	Numerical value 2	Label 3	Numerical value 3	Label 4	Numerical value 4
TEMP	T	100.	I	100.	T	600.	T	688.2
TEMP	T	700.	I	50.	T	900.	T	962.3
TEMP	T	1000.						

The temperature 298.15 K is always inserted in the temperature schedule automatically by PAC91 when there are temperature values below and above 298.15 K. (See examples 1 and 4, appendix D.)

If there are no TEMP records in a set of data where the thermodynamic functions are to be calculated, the program assumes the standard temperature schedule used in reference 4—namely, every 100 K from 100 to 6000 K with 298.15 K inserted between 200 and 300 K. (See example 7, appendix D.)

TEMP records should not precede METHOD records with READIN. For this option, the temperatures are read in on the data records together with the thermodynamic functions to which they correspond. (See examples 3, 6, and 8, appendix D.)

Appendix C—Details in Output

Listed Output

Input data in the uniform format as well as some intermediate data are listed for each set of input. Other tables and data will be listed according to the options on the OUTPUT record.

Input data.—All input data in the uniform format are listed immediately after they are read in the same format. Numerical values which are zero may be left blank. (See examples in appendix D.)

Tables of original thermodynamic properties.—(See section **Output** for discussion of original data and data from least-squares coefficients.) There are 10 possible tables printed according to the labels on the OUTPUT record, five for *original* data and a corresponding five for data calculated from least-squares coefficients. In each set of five tables, there are three possible many-figured tables (label MFIG) and two possible rounded tables with $\Delta_f H^o_T$ and $\log_{10}K$ columns (label LOGK). These tables vary with units: (1) dimensionless with DMLESS label (for many-figured tables only); (2) SI units with a JOULES label; and (3) energy units in calories with the CAL label. The properties in these tables are the following:

(1) In dimensionless form—

T, C^o_p/R, $(H^o_T - H^o_0)/RT$, $(H^o_T - H^o_{298.15})/RT$ (if T = 298.15 K is in T range), S^o_T/R, $-(G^o_T - H^o_0)/RT$, $-(G^o_T - H^o_{298.15})/RT$ (if T = 298.15 K is in T range), and H^o_T/RT and $-G^o_T/RT$ (if an H^o_0 value is available)

(2) In dimensioned, many-figured form—

T, C^o_p, $H^o_T - H^o_0$, $H^o_T - H^o_{298.15}$ (if T = 298.15 K is in T range), S^o_T, $-(G^o_T - H^o_0)$, $-(G^o_T - H^o_{298.15})$ (if T = 298.15 K is in T range), and H^o_T and $-G^o_T/RT$ (if an H^o_0 value is available)

(3) In dimensioned, rounded figure form—

T, C^o_p, $H^o_T - H^o_{298.15}$ (if T = 298.15 K is in T range), S^o_T, $-(G^o_T - H^o_{298.15})$ (if T = 298.15 K is in T range), H^o_T, and $\Delta_f H^o_T$ and $\log_{10}K$ for formation from assigned reference elements

These tables will have an asterisk and a footnote indicating where a phase transition has occurred in an assigned reference element. (See example 8, appendix D.)

All five of the tables containing original data have the word ORIGINAL on the bottom of each page.

Tables of thermodynamic properties from least-squares coefficients.—If a CTAB label is included on an OUTPUT record, tables of properties calculated from least-squares coefficients will be listed. These tables will have the same format as the *original* tables described in the previous section for the same labels on the OUTPUT records. They may be differentiated from the tables of *original* data by the word COEFFICIENTS on the bottom of each page. The temperature schedule for these tables may be changed from the input temperature schedule by the use of CTEM records.

Tables of least-squares errors.—A least-squares fit of the functions C^o_p/R, $(H^o_T - H^o_0)/RT$, and S^o_T/R results when a LSQS label is included on the OUTPUT record. (See examples 1, 6, 7, and 8 in appendix D.)

For each temperature interval, the following information is listed:

(1) For each T within the interval,
  (a) C^o_p/R, $(H^o_T - H^o_0)/RT$, S^o_T/R, and $-(G^o_T - H^o_0)/RT$
  (b) Functions in (1a) above as calculated from least-squares coefficients and equations (11) to (13)
  (c) Differences in (1a) and (1b); these values are referred to as errors hereinafter
  (d) Values in (1c) divided by original values in (1a); these values are referred to as relative errors hereinafter

(2) For errors in entire interval for each function in (1a):
  (a) Maximum relative error (MAX REL ERR) and corresponding temperature—see (1d)
  (b) Average relative error (AVER REL ERR)—see (1d)
  (c) Root mean square of relative errors (REL LST SQ ERR)—see (1d)
  (d) Maximum error (MAX ERR) and corresponding temperature—see (1c)
  (e) Average error (AVER ERR)—see (1c)
  (f) Root mean square of errors (LST SQ ERR)—see (1c)
  (g) C^o_p/R equation (see eq. (11)) for coefficients a_i
  (h) Integration constants in equations (12) and (13) as follows:

$$(H - H0)/R \text{ CONSTANT} = b_1 - H^o_0/R$$

$$H/R \text{ CONSTANT} = b_1$$
$$S/R \text{ CONSTANT} = b_2$$

Finally, the contents of the least-squares coefficient records are listed on I/O unit 10 as well as on I/O unit 6. See the section **Output** and table VIII.

EF data.—These data, which contain the enthalpy and Gibbs energy data for reference elements, will be listed for two situations. First, they will be listed when a reference element is being processed and there is an EFTAPE label on the OUTPUT record. The data, in dimensionless form, are written on I/O unit 11 as well as on I/O unit 6 (see example 6, Appendix D for a listing of EF data for a reference element). The data are also merged in the library of unformatted data on I/O unit 13 (see **Saved Output**). Secondly, a LISTEF record will cause all unformatted data on I/O unit 13 to be listed.

Intermediate data with FILL option for monatomic gases.—Unobserved but predicted energy levels for monatomic gases will be included in the partition function (eq. (7)) if the FILL code is included in the METHOD record. See the section **Inclusion of predicted levels** for the method of predicting the levels.

In argon (example 1, appendix D), the following data are listed in columns from left to right (refer to eq. (8) and table I):

(1) b value
(2) Principal quantum number n
(3) bn^2 or c^* [predicted $\Sigma\ (2J_i + 1)$]
(4) $\Sigma\ (2J_i + 1)$ from input data
(5) Column (3) minus column (4)
(6) Highest energy level for principal quantum number
(7) Sum of column (5) and $2J_i + 1$ for level of column (6)

Intermediate data with INTERM label.—Intermediate data are listed for ideal gas calculations if an INTERM label is included on the OUTPUT record for a particular species.

Monatomic gases: For monatomic gases several items are listed. The input data are listed in order of increasing energy level values. The data include, from left to right, values for the principal quantum number n, J_i, $2J_i + 1$, and the energy level.

For each temperature, three lines of data are listed as follows:

(1) A statement indicating where the energy levels were cut off; five possible statements are the following:

(a) NOT ALL LEVELS WERE USED. X IS GREATER THAN 85.—This statement indicates that not all atomic energy levels were used because $\epsilon/kT > 85$ in equation (7).

(b) ALL LEVELS USED THROUGH N = (FIXEDN value)—This statement indicates all atomic levels were used through a fixed principal quantum number (method FIXEDN).

(c) ALL ASSIGNED LEVELS HAVE BEEN USED—This statement indicates all atomic levels in input were used (method ALLN).

(d) NOT ALL ASSIGNED LEVELS WERE USED, Q AND DERIVATIVES ARE TOO SMALL—This statement indicates not all atomic levels were used because the following conditions occurred:

$$Q^m \leq 1 \times 10^{-10}$$

and

$$(\epsilon_m/kT)^2 Q^m \leq 1 \times 10^{-10}$$

when $\epsilon_m/kT > 2$.

(e) ALL LEVELS HAVE BEEN USED TO THE THERMAL BINDING ENERGY—This statement gives the lowered ionization potential value (i.e., ionization potential—kT/hc) where energy levels with higher values have been cut off.

(2) Values of T, C_p^o/R, $(H_T^o - H_0^o)/RT$, and $-(G_T^o - H_0^o)/RT$

(3) Values of ϵ/kT, Q, $T\,dQ/dT$, $T^2\,d^2Q/dT^2 + 2T\,dQ/dT$

Diatomic and polyatomic gases: Intermediate results are listed when an INTERM record is included in the input data set for a diatomic or polyatomic gas and the method of calculation is RRHO, JANAF, PANDK, NRRAO1, or NRRAO2. These results include values for the formulas and variables defined in tables II and III. Although the molecular constants are always listed as they appear in the data records, with an INTERM record many of them are listed again.

The following data are listed (see tables II and III for definitions and $H_2O(g)$ in example 5, appendix D):

(1) a_i, α_i^A, α_i^B, α_i^C where $i = 1$ to the number of unique frequencies
(2) θ_1, θ_2, θ_3
(3) A_0, B_0, C_0, ρ
(4) y_{ijk}
(5) x_{ij}
(6) LEVEL = (value in record columns 79 to 80 which is used to identify the electronic levels)
(7) ν_i, d_i, g_{ii}
(8) T
(9) u_i, r_i, s_i, i
(10) As required by the method of calculation, values for the formulas in tables II and III are listed for Q, ln Q, $T\,d(\ln Q)/dT$, and $T^2\,d^2(\ln Q)/dT^2 + 2T\,d(\ln Q)/dT$. The latter three values are additive contributions to $-(G_T^o - H_0^o)/RT$, $(H_T^o - H_0^o)/RT$, and C_p^o/R, respectively, when only the ground electronic state is considered. These values are identified in the listing by codes which correspond to the formula numbers as follows:

Code on listing	Formula numbers in tables II and III
ELEC	1
H.O.	2
R.R.	3 or 4
RHO	5
THTA	6
FERM	7
ALFA	8 to 11
XIJ	12 or 14
YIJK	13
G+AG	16
WEZE	15
AXIJ	17
XIJ2	18 and 19
XY	20 and 21
G2GX	22 and 23
AX2	24 to 27

Saved Output

As previously mentioned (see section **Computer Program**), some of the options require I/O units 10, 11, 13, 14, 17, and 19 in addition to the standard I/O units 5 and 6. I/O units 14 and 17 are scratch formatted and unformatted output units respectively for EF data processing. The other I/O units

contain data that may be saved for various purposes as summarized in the following table. More details are given in the following sections.

I/O unit[a]	Option		Contents	Format	I/O type
	Record ID	Label			
10	OUTPUT	LSQS	Coefficients (Groups and Species)	Formatted (table VIII)	Output
19	METHOD	ADD	Coefficients (Group)	Formatted (table VIII)	Input
13	OUTPUT	EFTAPE	EF data[b]	Unformatted	Output
11	OUTPUT	EFTAPE	EF data[b]	Formatted	Output
13	OUTPUT	LOGK	EF data[b]	Unformatted	Input
5	EFDA	(element)	EF data[b]	Formatted	Input

[a]Note that some of the input data (I/O units 19, 13, and 5) used by PAC91 were also produced by PAC91 (I/O units 10, 13, and 11).
[b]Reference elements.

The coefficients for a group written on I/O unit 10 have to be moved to the file associated with I/O unit 19 for future use. On the other hand, when an EFTAPE label is included on the OUTPUT record for a reference element, the EF data are automatically inserted in the unformatted data on I/O unit 13 for immediate use. The data are also written in formatted form on unit 11 which may be moved to a file as a backup. This file may be read in on I/O unit 5 and the program will put the data on I/O unit 13. The LISTEF record simply lists the data from I/O unit 13 so that they may be checked if so desired.

EF data.—For every reference element processed by PAC91 which includes an EFTAPE label on the OUTPUT record, the EF data which are generated are stored in I/O unit 11 in formatted form and in I/O unit 13 in unformatted form. (See example 6, appendix D, for a typical EF data set.) I/O unit 11 is used to store these data for just the reference elements currently being processed. I/O unit 13, by contrast, is used to include these data with EF data for all reference elements previously processed. If the current element has the same name as an element previously stored on I/O unit 13, the previously stored data for that element will be replaced by the current data. The formatted data on I/O unit 11 may be moved to another file and saved if desired. There are three reasons for doing this: (1) the data are legible, (2) they can serve as a backup since PAC91 can read in the data on I/O unit 5 and write it out on I/O unit 13, and (3) they are more easily transported to other computer systems.

Least-squares coefficients.—The least-squares coefficients are written in the file associated with I/O unit 10. The format is described in table VIII. Generally these data will be for use in other computer programs (e.g., ref. 41). These coefficients may also be for a group and used by PAC91 for the group additivity method (METHOD ADD). For this latter case, the coefficients must be transferred from I/O unit 10 to the file of data associated with I/O unit 19.

Appendix D—Examples

Eight sample problems were selected to illustrate a number of the methods, features, and options of PAC91. Both input and output are given in these examples. To conserve space, the output has been deliberately kept short by using shorter temperature schedules than would normally be used. For example, only one temperature, $T = 5000$ K, is given for H_2O due to the large amount of intermediate output.

In addition to the H_2O intermediate output several other types of intermediate output are also illustrated. These will be discussed for the appropriate examples.

The following methods are illustrated for the species shown:

Method	Species	Example numbers
ADD	C_2H_3	2
COEF	$Mg(\ell)$, $Na_2CO_3(\ell)$	6,8
JANAF	MgO	7
NRRAO2	H_2O	5
READIN	C_4H_4, Mg(s), Na_2CO_3(1,2)	3,6,8
RRHO	C_5H_{11}	4
TEMPER	Ar	1
WILH	C_2H_3, C_4H_4	2,3

The required records—namely, the formula, OUTPUT, METHOD, data and FINISH records—appear in each example. The optional NAME, DATE, REFNCE, TEMP, and CTEM records as well as a number of other records and labels are also illustrated in the following examples.

Example 1. Ar(g) from Method TEMPER with FILL and LSQS Options

Problem.—Calculate and print thermodynamic functions to 20 000 K for Ar using method TEMPER with FILL option and obtain a least-squares fit of the calculated data. Print tables of functions, both original data and data from least-squares coefficients, in the three options of energy units and the many-figured form.

The standard I/O unit 5 input and the standard I/O unit 6 output are listed below.

For the input, the record names were all limited to four characters except the FINISH record. The number of and names of these records are, in order: 1 NAME, 1 formula, 1 DATE, 1 REFN, 2 TEMP, 5 LSTS, 2 OUTP, 1 METH, 35 data, and 1 FINISH. The NAME record gives the name of the species and, for the comments portion, the data reference and method of calculation. The formula record gives the species formula in capital letters for the alphabetic part, the stoichiometric coefficient of 1, and the assigned enthalpy of 0 at 298.15 K (HF298). The DATE record contains a code chosen to stand for Lewis, June 1988—namely, L 6/88. The REFN record gives more information regarding the reference for the spectroscopic data. The TEMP records give the temperature schedule—namely, 100 and 500 and 1000 to 20 000 K in 1000 K increments. The first LSTS record gives the temperature interval endpoints for the least-squares fit—namely, 298.15, 1000, 6000, and 20 000 K. The second and third LSTS records give just one EXP = 0 value (q_i in eq. (11)) for temperatures intervals 1 and 2 (given in column 80). This is because C_p^o/R is a constant in these temperature ranges. The last two LSTS records give seven exponent values for the third interval (6000 to 20 000 K).

No least-squares fitting will take place and no tables printed unless these options are listed on the OUTP records. In this case, the options include many-figured tables (MFIG) in three sets of energy units (DMLESS, JOULES, and CAL), a least-squares fit (LSQS), and tables from the least-squares coefficients (CTAB). Specified energy units apply to both original and least-squares tables.

The METH record indicates the temperature cutoff method (TEMPER) with the missing levels filled in (FILL). The data records, which are identified by AR in columns 1 and 2, contain energy levels and corresponding J_m values. The principal quantum numbers 3 through 14 to which these energy levels belong are required by FILL and are given in columns 79 and 80. The J_m values are found in the label portions of the records. Note that these values may be anywhere in the label columns and integers do not require decimal points. The last data record contains the ionization potential (IP) needed for the temperature cutoff method.

The first part of the listed output is simply a copy of the input records except for the atomic weight which is inserted after the METH record. The seven columns of information following the FINISH record are related to the FILL option. These are described in appendix C under **Intermediate data with FILL option for monatomic gases**. Similarly, the least-squares output is detailed in the section **Tables of least-squares errors**. The remaining tables result from the remaining labels on the OUTP record—namely, DMLESS, JOULES, CAL, MFIG, and CTAB. Again refer to the appendix C sections **Tables of original thermodynamic properties** and **Tables of thermodynamic properties from least-squares coefficients**.

Input. - The input data set for Ar, example 1, is as follows:

	Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	Argon		NSRDS-	NBS 35, 1971	. Temperature cutoff & FILL. Expl.				1
	AR1			HF298	0.					
	DATE	L 6/88								
a	REFN	MOORE,	ATOMIC ENERGY LEVELS, NSRDS-NBS 35,				1971, PP 21	1-215.		
	TEMP	T	100.	T	500.	T	1000.	I	1000.	
	TEMP	T	20000.							
	LSTS	T	298.15	T	1000.	T	6000.	T	20000.	
	LSTS	EXP	0.							1
	LSTS	EXP	0.							2
	LSTS	EXP	0.	EXP	1.	EXP	2.	EXP	3.	3
	LSTS	EXP	4.	EXP	-1.	EXP	-2.			3
	OUTP	MFIG		DMLESS		JOULES		CAL		
	OUTP	LSQS		CTAB						
	METH	TEMPER		FILL						
	AR	0	0.	0	111667.87					3
	AR	1	111818.09	4	112750.22	3	113020.39	2	112138.98	3
	AR	1	114147.75	2	113426.05	3	113716.61	2	114641.04	3
	AR	3	114831.99	2	114805.18	1	115366.9			3
	AR			2	93143.8	1	93750.639	0	94553.707	4
	AR	1	95399.87	1	104102.144	3	105462.804	2	105617.315	4
	AR	1	106087.305	2	106237.597	0	107054.319	1	107131.755	4
	AR	2	107289.747	1	107496.463	0	108722.668			4
	AR	0	118512.17	1	118651.447	4	119023.699	3	119212.93	4
	AR	2	118906.665	1	119847.81	2	119444.88	3	119566.11	4
	AR	2	120619.076	3	120753.52	2	120600.944	1	121011.979	4
	AR	1	120188.34	2	120188.66	5	120207.32	4	120207.77	4
	AR	3	120229.81	2	120230.07	7.5	120250.15	13.5	121654.	4
	AR	2	113468.55	1	113643.26	0	114861.67	1	114975.07	5
	AR	1	116660.054	3	116942.815	2	116999.389	1	117151.387	5
	AR	2	117183.654	0	117563.020	1	118407.494	2	118469.117	5
	AR	1	118459.662	0	118870.981	0	121794.158	1	121932.908	5
	AR	10	122090.	1	122514.29	5.5	122310.	5.5	123535.	5
	AR	2	123372.987	1	123815.53	27.5	122700.	13.5	124137.	5
	AR	2	119683.113	1	119760.22	0	121096.67	1	121161.356	6
	AR	11.5	121205.	5.5	122633.	19.5	123741.	9.5	125140.	6
	AR	27.5	124050.	13.5	125483.					6
	AR	3.5	122455.	1.5	123880.	11.5	123230.	5.5	124660.	7
	AR	19.5	124652.	9.5	126069.	27.5	124863.	13.5	126295.	7
	AR	11.5	124400.	5.5	125800.	19.5	125280.	27.5	125390.	8
	AR	3.5	123920.	1.5	125340.					8
	AR	3.5	124780.	1.5	126210.	11.5	125100.	1.5	126524.2	9
	AR	19.5	125650.	3.5	127130.	27.5	125754.			9
	AR	3.5	125330.	11.5	125540.	19.5	125940.	3.5	127410.	10
	AR	3.5	125712.	1.5	127130.	5.5	125860.	19.5	126155.	11
	AR	3.5	127610.							11
	AR	7.5	126000.	19.5	126300.	3.5	127760.			12
	AR	5.5	126200.	1.5	127610.	19.5	126430.	3.5	127880.	13
	AR	3.5	126330.	1.5	127600.	19.5	126520.	3.5	127970.	14
	AR	IP	127109.9							
	FINISH									

[a]All alphanumeric characters.

Listed output. - The listed output for Ar, example 1, is as follows:

```
NAME  Argon              NSRDS-NBS 35, 1971. Temperature cutoff & FILL.   Expl. 1
AR1                      HF298    0.
DATE  L 6/88
REFN  MOORE, ATOMIC ENERGY LEVELS, NSRDS-NBS 35, 1971, PP 211-215.
TEMP  T      100.        T       500.       T      1000.       I        1000.
TEMP  T    20000.
LSTS  T      298.15      T      1000.       T      6000.       T       20000.
LSTS  EXP      0.                                                             1
LSTS  EXP      0.                                                             2
LSTS  EXP      0.        EXP      1.        EXP       2.       EXP       3.  3
LSTS  EXP      4.        EXP     -1.        EXP      -2.                       3
OUTP  MFIG               DMLESS             JOULES             CAL
OUTP  LSQS               CTAB
METH  TEMPER             FILL
ATOMIC WEIGHT =  39.94800
AR     0          0.     0      111667.87                                     3
AR     1     111818.09   4      112750.22  3      113020.39  2      112138.98  3
AR     1     114147.75   2      113426.05  3      113716.61  2      114641.04  3
AR     3     114831.99   2      114805.18  1      115366.9                     3
AR                       2       93143.8   1       93750.639 0       94553.707 4
AR     1      95399.87   1      104102.144 3       105462.804   2    105617.315 4
AR     1     106087.305  2      106237.597 0       107054.319 1      107131.755 4
AR     2     107289.747  1      107496.463 0       108722.668                   4
AR     0     118512.17   1      118651.447 4       119023.6993       119212.93  4
AR     2     118906.665  1      119847.81  2       119444.88  3      119566.11  4
AR     2     120619.076  3      120753.52  2       120600.944 1      121011.979 4
AR     1     120188.34   2      120188.66  5       120207.32  4      120207.77  4
AR     3     120229.81   2      120230.07  7.5     120250.15  13.5   121654.    4
AR     2     113468.55   1      113643.26  0       114861.67  1      114975.07  5
AR     1     116660.054  3      116942.815 2       116999.389 1      117151.387 5
AR     2     117183.654  0      117563.020 1       118407.494 2      118469.117 5
AR     1     118459.662  0      118870.981 0       121794.158 1      121932.908 5
AR     10    122090.     1      122514.29  5.5     122310.    5.5    123535.    5
AR     2     123372.987  1      123815.53  27.5    122700.    13.5   124137.    5
AR     2     119683.113  1      119760.22  0       121096.67  1      121161.356 6
AR     11.5  121205.     5.5    122633.    19.5    123741.    9.5    125140.    6
AR     27.5  124050.     13.5   125483.                                       6
AR     3.5   122455.     1.5    123880.    11.5    123230.    5.5    124660.    7
AR     19.5  124652.     9.5    126069.    27.5    124863.    13.5   126295.    7
AR     11.5    124400.   5.5     125800.   19.5    125280.    27.5   125390.    8
AR     3.5   123920.     1.5     125340.                                       8
AR     3.5   124780.     1.5    126210.    11.5    125100.    1.5    126524.2   9
AR     19.5   125650.    3.5     127130.   27.5    125754.                     9
AR     3.5   125330.     11.5     125540.  19.5    125940.    3.5    127410.    10
AR     3.5   125712.     1.5    127130.    5.5     125860.    19.5   126155.    11
AR     3.5   127610.                                                          11
AR     7.5    126000.    19.5    126300.   3.5     127760.                     12
AR     5.5    126200.    1.5    127610.    19.5     126430.   3.5     127880.  13
AR     3.5   126330.     1.5    127600.    19.5    126520.    3.5    127970.    14
AR     IP     127109.9

FINISH
      B          N   PRED. SUM(2J+1)   ACT. SUM(2J+1)   DIFF     MAX LEVEL   2J+1, MAX LEVEL
    12.0         3          61.0             61.0        0.0    115366.9000        3.0
    12.0         4         192.0            192.0        0.0    121654.0000       28.0
    12.0         5         300.0            192.0      108.0    124137.0000      136.0
    12.0         6         432.0            192.0      240.0    125483.0000      268.0
    12.0         7         588.0            192.0      396.0    126295.0000      424.0
    12.0         8         768.0            144.0      624.0    125800.0000      636.0
    12.0         9         972.0            144.0      828.0    127130.0000      836.0
    12.0        10        1200.0             80.0     1120.0    127410.0000     1128.0
    12.0        11        1452.0             72.0     1380.0    127610.0000     1388.0
    12.0        12        1728.0             64.0     1664.0    127760.0000     1672.0
    12.0        13        2028.0             64.0     1964.0    127880.0000     1972.0
    12.0        14        2352.0             60.0     2292.0    127970.0000     2300.0

                                BAR    Argon
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LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
298.15	2.5000000	2.5000000	2.5000000	2.5000000	18.6236667	18.6236667	16.1236667	16.1236667
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
500.00	2.5000000	2.5000000	2.5000000	2.5000000	19.9161952	19.9161952	17.4161952	17.4161952
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
1000.00	2.5000000	2.5000000	2.5000000	2.5000000	21.6490631	21.6490631	19.1490631	19.1490631
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000

MAX REL ERR CP/R = 0.000000 TEMP = 1000. AVER REL ERR CP/R = 0.000000 REL LST SQ ERR CP/R = 0.000000
MAX REL ERR HH/RT = 0.000000 TEMP = 298. AVER REL ERR HH/RT = 0.000000 REL LST SQ ERR HH/RT = 0.000000
MAX REL ERR S/R = 0.000000 TEMP = 500. AVER REL ERR S/R = 0.000000 REL LST SQ ERR S/R = 0.000000
MAX REL ERR GH/RT = 0.000000 TEMP = 500. AVER REL ERR GH/RT = 0.000000 REL LST SQ ERR GH/RT = 0.000000
MAX ERR CP/R = 0.000000 TEMP.= 1000. AVER ERR CP/R = 0.000000 LST SQ ERR CP/R = 0.000000
MAX ERR HH/RT = 0.000000 TEMP = 298. AVER ERR HH/RT = 0.000000 LST SQ ERR HH/RT = 0.000000
MAX ERR S/R = 0.000000 TEMP = 500. AVER ERR S/R = 0.000000 LST SQ ERR S/R = 0.000000
MAX ERR GH/RT = 0.000000 TEMP = 500. AVER ERR GH/RT = 0.000000 LST SQ ERR GH/RT = 0.000000

CP/R = 2.5000000e+00T** 0.0
(H-H0)/R CONSTANT = -0.11368684e-12, H/R CONSTANT =-0.74537500e+03, S/R CONSTANT = 0.43796749e+01

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
1000.00	2.5000000	2.5000000	2.5000000	2.5000000	21.6490631	21.6490631	19.1490631	19.1490631
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
2000.00	2.5000000	2.5000000	2.5000000	2.5000000	23.3819311	23.3819311	20.8819311	20.8819311
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
3000.00	2.5000000	2.5000000	2.5000000	2.5000000	24.3955938	24.3955938	21.8955938	21.8955938
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
4000.00	2.5000000	2.5000000	2.5000000	2.5000000	25.1147990	25.1147990	22.6147990	22.6147990
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
5000.00	2.5000000	2.5000000	2.5000000	2.5000000	25.6726579	25.6726579	23.1726579	23.1726579
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
6000.00	2.5000014	2.5000000	2.5000001	2.5000000	26.1284618	26.1284618	23.6284618	23.6284613
	0.0000014	0.0000006	0.0000001	0.0000000	0.0000001	0.0000000	0.0000000	0.0000000

MAX REL ERR CP/R = 0.000001 TEMP = 6000. AVER REL ERR CP/R = 0.000000 REL LST SQ ERR CP/R = 0.000000
MAX REL ERR HH/RT = 0.000000 TEMP = 6000. AVER REL ERR HH/RT = 0.000000 REL LST SQ ERR HH/RT = 0.000000
MAX REL ERR S/R = 0.000000 TEMP = 6000. AVER REL ERR S/R = 0.000000 REL LST SQ ERR S/R = 0.000000
MAX REL ERR GH/RT = 0.000000 TEMP = 6000. AVER REL ERR GH/RT = 0.000000 REL LST SQ ERR GH/RT = 0.000000
MAX ERR CP/R = 0.000001 TEMP.= 6000. AVER ERR CP/R = 0.000000 LST SQ ERR CP/R = 0.000001
MAX ERR HH/RT = 0.000000 TEMP = 6000. AVER ERR HH/RT = 0.000000 LST SQ ERR HH/RT = 0.000000
MAX ERR S/R = 0.000000 TEMP = 6000. AVER ERR S/R = 0.000000 LST SQ ERR S/R = 0.000000
MAX ERR GH/RT = 0.000000 TEMP = 6000. AVER ERR GH/RT = 0.000000 LST SQ ERR GH/RT = 0.000000

CP/R = 2.5000000e+00T** 0.0
(H-H0)/R CONSTANT = -0.34106051e-12, H/R CONSTANT =-0.74537500e+03, S/R CONSTANT = 0.43796749e+01

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
6000.00	2.5000014	2.5000000	2.5000001	2.5000000	26.1284618	26.1284618	23.6284618	23.6284613
	0.0000014	0.0000006	0.0000001	0.0000000	0.0000001	0.0000000	0.0000000	0.0000000
7000.00	2.5000300	2.4949369	2.5000015	2.5003617	26.5138400	26.5142450	24.0138386	24.0138833
	0.0050931	0.0020372	-0.0003602	-0.0001441	-0.0004050	-0.0000153	-0.0000448	-0.0000019
8000.00	2.5003059	2.4836759	2.5000167	2.4987464	26.8476846	26.8464133	24.3476679	24.3476669
	0.0166300	0.0066512	0.0012704	0.0005081	0.0012713	0.0000474	0.0000009	0.0000000
9000.00	2.5018654	2.4912337	2.5001131	2.4973788	27.1422446	27.1392646	24.6421315	24.6418853
	0.0106317	0.0042495	0.0027343	0.0010937	0.0029801	0.0001098	0.0002457	0.0000103
10000.00	2.5074146	2.5047161	2.5004979	2.4974261	27.4060574	27.4024269	24.9055595	24.9050009
	0.0026985	0.0010762	0.0030718	0.0012285	0.0036305	0.0001325	0.0005587	0.0000224
11000.00	2.5234699	2.5210257	2.5017210	2.4987833	27.6456495	27.6418679	25.1439285	25.1430845
	0.0024441	0.0009686	0.0029377	0.0011743	0.0037817	0.0001368	0.0008439	0.0000336
12000.00	2.5588346	2.5512414	2.5046980	2.5017379	27.8664056	27.8623567	25.3617076	25.3606187
	0.0075932	0.0029674	0.0029601	0.0011818	0.0040489	0.0001453	0.0010888	0.0000429
13000.00	2.6274245	2.6146798	2.5110032	2.5077049	28.0733960	28.0687779	25.5623928	25.5610730
	0.0127447	0.0048506	0.0032982	0.0013135	0.0046181	0.0001645	0.0013198	0.0000516
14000.00	2.7520110	2.7316496	2.5233415	2.5191514	28.2722222	28.2664413	25.7488807	25.7472899
	0.0203613	0.0073987	0.0041901	0.0016605	0.0057809	0.0002045	0.0015908	0.0000618
15000.00	2.9194142	2.9171869	2.5418264	2.5390956	28.4652037	28.4608115	25.9233774	25.9217159
	0.0022273	0.0007629	0.0027308	0.0010743	0.0043923	0.0001543	0.0016615	0.0000641
16000.00	3.1811838	3.1761285	2.5725349	2.5704448	28.6608111	28.6569628	26.0882763	26.0865180
	0.0050553	0.0015891	0.0020901	0.0008125	0.0038484	0.0001343	0.0017583	0.0000674
17000.00	3.5296303	3.4993640	2.6169087	2.6153123	28.8622713	28.8589372	26.2453625	26.2436249
	0.0302663	0.0085749	0.0015964	0.0006100	0.0033341	0.0001155	0.0017376	0.0000662
18000.00	3.8183774	3.8610148	2.6607190	2.6743812	29.0552237	29.0690987	26.3945047	26.3947176
	-0.0426374	-0.0111664	-0.0136621	-0.0051348	-0.0138751	-0.0004775	-0.0002129	-0.0000081
19000.00	4.2690023	4.2163096	2.7297792	2.7463394	29.2695115	29.2875293	26.5397323	26.5411899
	0.0526927	0.0123431	-0.0165602	-0.0060665	-0.0180178	-0.0006156	-0.0014576	-0.0000549
20000.00	4.4885984	4.4999787	2.7773394	2.8273923	29.4538747	29.5114850	26.6765353	26.6840927
	-0.0113803	-0.0025354	-0.0500529	-0.0180219	-0.0576103	-0.0019559	-0.0075573	-0.0002833

MAX REL ERR CP/R = 0.012343 TEMP = 19000. AVER REL ERR CP/R = 0.004478 REL LST SQ ERR CP/R = 0.005864
MAX REL ERR HH/RT = 0.018022 TEMP = 20000. AVER REL ERR HH/RT = 0.002668 REL LST SQ ERR HH/RT = 0.005166
MAX REL ERR S/R = 0.001956 TEMP = 20000. AVER REL ERR S/R = 0.000294 REL LST SQ ERR S/R = 0.000555
MAX REL ERR GH/RT = 0.000283 TEMP = 20000. AVER REL ERR GH/RT = 0.000051 REL LST SQ ERR GH/RT = 0.000084
MAX ERR CP/R = 0.052693 TEMP.= 19000. AVER ERR CP/R = 0.014830 LST SQ ERR CP/R = 0.021188
MAX ERR HH/RT = 0.050053 TEMP = 20000. AVER ERR HH/RT = 0.007168 LST SQ ERR HH/RT = 0.014248
MAX ERR S/R = 0.057610 TEMP = 20000. AVER ERR S/R = 0.008506 LST SQ ERR S/R = 0.016311
MAX ERR GH/RT = 0.007557 TEMP = 20000. AVER ERR GH/RT = 0.001339 LST SQ ERR GH/RT = 0.002232

CP/R = -1.2955921e+09T**-2.0 8.2201459e+05T**-1.0 -2.0865673e+02T** 0.0 2.8064385e-02T** 1.0 -2.0298347e-06T** 2.0
7.5268416e-11T** 3.0 -1.1012887e-15T** 4.0
(H-H0)/R CONSTANT = -0.64818047e+07, H/R CONSTANT =-0.64825501e+07, S/R CONSTANT = 0.18234371e+04

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

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Argon             NSRDS-NBS 35, 1971. Temperature cutoff & FILL.   Expl. 1
 3 L 6/88 AR  1.00    0.00    0.00    0.00    0.00 0      39.94800          0.000
    298.150  1000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0          6197.428
  2.50000000d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -7.45375000d+02  4.37967491d+00
   1000.000  6000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0          6197.428
  2.50000000d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -7.45375000d+02  4.37967491d+00
   6000.000 20000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          6197.428
 -1.29559206d+09  8.22014586d+05 -2.08656731d+02  2.80643848d-02 -2.02983469d-06
  7.52684157d-11 -1.10128867d-15  0.00000000d+00 -6.48255009d+06  1.82343707d+03
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ORIGINAL BAR Argon

ORIGINAL Argon

ASSIGNED H/R AT 0 K = -745.375 K

T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
100.00	2.50000	2.5000000	-4.9537500	15.8926004	13.3926004	20.8463504	-4.9537500	20.8463504
298.15	2.50000	2.5000000	0.0000000	18.6236667	16.1236667	18.6236667	0.0000000	18.6236667
500.00	2.50000	2.5000000	1.0092500	19.9161952	17.4161952	18.9069452	1.0092500	18.9069452
1000.00	2.50000	2.5000000	1.7546250	21.6490631	19.1490631	19.8944381	1.7546250	19.8944331
2000.00	2.50000	2.5000000	2.1273125	23.3819311	20.8819311	21.2546186	2.1273125	21.2546186
3000.00	2.50000	2.5000000	2.2515417	24.3955938	21.8955938	22.1440522	2.2515417	22.1440522
4000.00	2.50000	2.5000000	2.3136562	25.1147990	22.6147990	22.8011428	2.3136562	22.8011428
5000.00	2.50000	2.5000000	2.3509250	25.6726579	23.1726579	23.3217329	2.3509250	23.3217329
6000.00	2.50000	2.5000001	2.3757709	26.1284618	23.6284618	23.7526910	2.3757709	23.7526910
7000.00	2.50003	2.5000015	2.3935193	26.5138400	24.0138386	24.1203207	2.3935193	24.1203207
8000.00	2.50031	2.5000167	2.4068449	26.8476846	24.3476679	24.4408398	2.4068449	24.4408398
9000.00	2.50187	2.5001131	2.4172937	27.1422446	24.6421315	24.7249509	2.4172937	24.7249509
10000.00	2.50741	2.5004979	2.4259604	27.4060574	24.9055595	24.9800970	2.4259604	24.9800970
11000.00	2.52347	2.5017210	2.4339597	27.6456495	25.1439285	25.2116898	2.4339597	25.2116898
12000.00	2.55883	2.5046980	2.4425834	27.8664056	25.3617076	25.4238222	2.4425834	25.4238222
13000.00	2.62742	2.5110032	2.4536666	28.0733960	25.5623928	25.6197293	2.4536666	25.6197293
14000.00	2.75201	2.5233415	2.4701004	28.2722222	25.7488807	25.8021218	2.4701004	25.8021218
15000.00	2.91941	2.5418264	2.4921347	28.4652037	25.9233774	25.9730691	2.4921347	25.9730691
16000.00	3.18118	2.5725349	2.5259490	28.6608111	26.0882763	26.1348622	2.5259490	26.1348622
17000.00	3.52963	2.6169087	2.5730632	28.8622713	26.2453625	26.2892081	2.5730632	26.2892081
18000.00	3.81838	2.6607190	2.6193093	29.0552237	26.3945047	26.4359144	2.6193093	26.4359144
19000.00	4.26900	2.7297792	2.6905489	29.2695115	26.5397323	26.5789626	2.6905489	26.5789626
20000.00	4.48860	2.7773394	2.7400706	29.4538747	26.6765353	26.7138041	2.7400706	26.7138041

ORIGINAL Argon

ASSIGNED H AT 0 K = -6197.428 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
100.00	20.78627	2078.627	-4118.800	132.139185	11135.291	17332.719	-4118.800	17332.719
298.15	20.78627	6197.428	0.000	154.846663	39970.105	46167.533	0.000	46167.533
500.00	20.78627	10393.137	4195.710	165.593404	72403.564	78600.992	4195.710	78600.992
1000.00	20.78627	20786.275	14588.847	180.001352	159215.077	165412.505	14588.847	165412.505
2000.00	20.78627	41572.550	35375.122	194.409300	347246.049	353443.477	35375.122	353443.477
3000.00	20.78627	62358.825	56161.397	202.837409	546153.402	552350.829	56161.397	552350.829
4000.00	20.78628	83145.100	76947.672	208.817248	752123.890	758321.318	76947.672	758321.318
5000.00	20.78628	103931.375	97733.947	213.455571	963346.479	969543.907	97733.947	969543.907
6000.00	20.78629	124717.653	118520.225	217.245357	1178754.491	1184951.919	118520.225	1184951.919
7000.00	20.78652	145504.010	139306.582	220.449588	1397643.106	1403840.533	139306.582	1403840.533
8000.00	20.78882	166291.314	160093.886	223.225342	1619511.425	1625708.853	160093.886	1625708.853
9000.00	20.80179	187084.942	180887.514	225.674444	1843985.237	1850182.665	180887.514	1850182.665
10000.00	20.84792	207904.148	201706.720	227.867939	2070775.239	2076972.667	201706.720	2076972.667
11000.00	20.98142	228806.429	222609.002	229.860029	2299653.893	2305851.321	222609.002	2305851.321
12000.00	21.27546	249904.040	243706.612	231.695508	2530442.054	2536639.482	243706.612	2536639.482
13000.00	21.84575	271410.893	265213.465	233.416532	2763004.017	2769201.445	265213.465	2769201.445
14000.00	22.88162	293724.870	287527.442	235.069674	2997250.569	3003447.996	287527.442	3003447.996
15000.00	24.27350	317010.610	310813.182	236.674221	3233102.708	3239300.136	310813.182	3239300.136
16000.00	26.44998	342229.873	336032.445	238.300601	3470579.741	3476777.169	336032.445	3476777.169
17000.00	29.34715	369891.337	363693.909	239.975643	3709694.597	3715892.025	363693.909	3715892.025
18000.00	31.74794	398206.348	392008.920	241.579948	3950232.712	3956430.140	392008.920	3956430.140
19000.00	35.49466	431238.748	425041.321	243.361646	4192632.525	4198829.953	425041.321	4198829.953
20000.00	37.32050	461844.323	455646.895	244.894536	4436046.393	4442243.821	455646.895	4442243.821

ORIGINAL Argon

ASSIGNED H AT 0 K = -1481.221 CAL/MOLE

T DEG-K	CP CAL/MOL-K	H-H0 CAL/MOL	H-H298 CAL/MOL	S CAL/MOL-K	-(G-H0) CAL/MOL	-(G-H298) CAL/MOL	H CAL/MOL	-G CAL/MOL
100.00	4.96804	496.804	-984.417	31.582023	2661.398	4142.619	-984.417	4142.619
298.15	4.96804	1481.221	0.000	37.009241	9553.084	11034.305	0.000	11034.305
500.00	4.96804	2484.019	1002.799	39.577773	17304.867	18786.088	1002.799	18786.088
1000.00	4.96804	4968.039	3486.818	43.021356	38053.317	39534.537	3486.818	39534.537
2000.00	4.96804	9936.078	8454.857	46.464938	82993.798	84475.018	8454.857	84475.018
3000.00	4.96804	14904.117	13422.896	48.479304	130533.796	132015.017	13422.896	132015.017
4000.00	4.96804	19872.156	18390.935	49.908520	179761.924	181243.145	18390.935	181243.145
5000.00	4.96804	24840.195	23358.974	51.017106	230245.334	231726.555	23358.974	231726.555
6000.00	4.96804	29808.234	28327.014	51.922887	281729.085	283210.306	28327.014	283210.306
7000.00	4.96810	34776.293	33295.072	52.688716	334044.719	335525.940	33295.072	335525.940
8000.00	4.96865	39744.578	38263.357	53.352137	387072.520	388553.741	38263.357	388553.741
9000.00	4.97175	44714.374	43233.153	53.937491	440723.049	442204.270	43233.153	442204.270
10000.00	4.98277	49690.284	48209.063	54.461744	494927.160	496408.381	48209.063	496408.381
11000.00	5.01468	54686.049	53204.828	54.937866	549630.472	551111.692	53204.828	551111.692
12000.00	5.08496	59728.499	58247.278	55.376555	604790.166	606271.387	58247.278	606271.337
13000.00	5.22126	64868.760	63387.540	55.787890	660373.809	661855.030	63387.540	661855.030
14000.00	5.46884	70201.929	68720.708	56.183001	716360.079	717841.299	68720.708	717841.299
15000.00	5.80151	75767.354	74286.133	56.566496	772730.093	774211.314	74286.133	774211.314
16000.00	6.32170	81794.903	80313.682	56.955211	829488.466	830969.687	80313.682	830969.687
17000.00	7.01414	88406.151	86924.930	57.355555	886638.288	888119.509	86924.930	888119.509
18000.00	7.58794	95173.601	93692.381	57.738993	944128.277	945609.498	93692.381	945609.498
19000.00	8.48343	103068.535	101587.314	58.164829	1002063.223	1003544.444	101587.314	1003544.444
20000.00	8.91981	110383.442	108902.222	58.531199	1060240.534	1061721.755	108902.222	1061721.755

ORIGINAL BAR Argon

COEFFICIENTS Argon

ASSIGNED H/R AT 0 K = -745.375 K

T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
298.15	2.50000	2.5000000	0.0000000	18.6236667	16.1236667	18.6236667	0.0000000	18.6236667
500.00	2.50000	2.5000000	1.0092500	19.9161952	17.4161952	18.9069452	1.0092500	18.9069452
1000.00	2.50000	2.5000000	1.7546250	21.6490631	19.1490631	19.8944381	1.7546250	19.8944381
2000.00	2.50000	2.5000000	2.1273125	23.3819311	20.8819311	21.2546186	2.1273125	21.2546186
3000.00	2.50000	2.5000000	2.2515417	24.3955938	21.8955938	22.1440522	2.2515417	22.1440522
4000.00	2.50000	2.5000000	2.3136562	25.1147990	22.6147990	22.8011428	2.3136562	22.8011428
5000.00	2.50000	2.5000000	2.3509250	25.6726579	23.1726579	23.3217329	2.3509250	23.3217329
6000.00	2.50000	2.5000000	2.3757708	26.1284618	23.6284618	23.7526909	2.3757708	23.7526909
7000.00	2.49494	2.5003617	2.3938796	26.5142450	24.0138833	24.1203655	2.3938796	24.1203655
8000.00	2.48368	2.4987464	2.4055745	26.8464133	24.3476669	24.4408388	2.4055745	24.4408388
9000.00	2.49123	2.4973788	2.4145594	27.1392646	24.6418858	24.7247052	2.4145594	24.7247052
10000.00	2.50472	2.4974261	2.4228886	27.4024269	24.9050009	24.9795384	2.4228886	24.9795384
11000.00	2.52103	2.4987833	2.4310219	27.6418679	25.1430845	25.2108459	2.4310219	25.2108459
12000.00	2.55124	2.5017379	2.4396233	27.8623567	25.3606187	25.4227333	2.4396233	25.4227333
13000.00	2.61468	2.5077049	2.4503684	28.0687779	25.5610730	25.6184095	2.4503684	25.6184095
14000.00	2.73165	2.5191514	2.4659103	28.2664413	25.7472899	25.8005310	2.4659103	25.8005310
15000.00	2.91719	2.5390956	2.4894039	28.4608115	25.9217159	25.9714075	2.4894039	25.9714075
16000.00	3.17613	2.5704448	2.5238589	28.6569628	26.0865180	26.1331039	2.5238589	26.1331039
17000.00	3.49936	2.6153123	2.5714667	28.8589372	26.2436249	26.2874705	2.5714667	26.2874705
18000.00	3.86101	2.6743812	2.6329714	29.0690987	26.3947176	26.4361273	2.6329714	26.4361273
19000.00	4.21631	2.7463394	2.7071091	29.2875293	26.5411899	26.5804202	2.7071091	26.5804202
20000.00	4.49998	2.8273923	2.7901236	29.5114850	26.6840927	26.7213614	2.7901236	26.7213614

COEFFICIENTS Argon

ASSIGNED H AT 0 K = -6197.428 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
298.15	20.78627	6197.428	0.000	154.846663	39970.105	46167.533	0.000	46167.533
500.00	20.78627	10393.137	4195.710	165.593404	72403.564	78600.992	4195.710	78600.992
1000.00	20.78627	20786.275	14588.847	180.001352	159215.077	165412.505	14588.847	165412.505
2000.00	20.78627	41572.550	35375.122	194.409300	347246.049	353443.477	35375.122	353443.477
3000.00	20.78627	62358.825	56161.397	202.837409	546153.402	552350.829	56161.397	552350.829
4000.00	20.78627	83145.100	76947.672	208.817248	752123.890	758321.318	76947.672	758321.318
5000.00	20.78627	103931.375	97733.947	213.455571	963346.479	969543.907	97733.947	969543.907
6000.00	20.78627	124717.650	118520.222	217.245357	1178754.491	1184951.919	118520.222	1184951.919
7000.00	20.74418	145524.977	139327.549	220.452956	1397645.713	1403843.141	139327.549	1403843.141
8000.00	20.65055	166206.813	160009.385	223.214772	1619511.362	1625708.790	160009.385	1625708.790
9000.00	20.71339	186880.330	180682.902	225.649687	1843966.850	1850164.278	180682.902	1850164.278
10000.00	20.82549	207648.739	201451.311	227.837753	2070728.790	2076926.218	201451.311	2076926.218
11000.00	20.96109	228537.747	222340.319	229.828587	2299576.707	2305774.135	222340.319	2305774.135
12000.00	21.21232	249608.700	243411.272	231.661843	2530333.416	2536530.844	243411.272	2536530.844
13000.00	21.73978	271054.390	264856.962	233.378135	2762861.359	2769058.787	264856.962	2769058.787
14000.00	22.71233	293237.128	287039.701	235.021609	2997065.396	3003262.823	287039.701	3003262.823
15000.00	24.25498	316670.037	310472.609	236.637701	3232895.485	3239092.913	310472.609	3239092.913
16000.00	26.40795	341951.827	335754.399	238.268604	3470345.830	3476543.258	335754.399	3476543.258
17000.00	29.09550	369665.689	363468.261	239.947922	3709448.987	3715646.414	363468.261	3715646.414
18000.00	32.10245	400251.040	394053.612	241.695312	3950264.576	3956462.004	394053.612	3956462.004
19000.00	35.05655	433854.863	427657.435	243.511455	4192862.790	4199060.218	427657.435	4199060.218
20000.00	37.41512	470167.636	463970.208	245.373537	4437303.106	4443500.534	463970.208	4443500.534

COEFFICIENTS Argon

ASSIGNED H AT 0 K = -1481.221 CAL/MOLE

T DEG-K	CP CAL/MOL-K	H-H0 CAL/MOL	H-H298 CAL/MOL	S CAL/MOL-K	-(G-H0) CAL/MOL	-(G-H298) CAL/MOL	H CAL/MOL	-G CAL/MOL
298.15	4.96804	1481.221	0.000	37.009241	9553.084	11034.305	0.000	11034.305
500.00	4.96804	2484.019	1002.799	39.577773	17304.867	18786.088	1002.799	18786.088
1000.00	4.96804	4968.039	3486.818	43.021356	38053.317	39534.537	3486.818	39534.537
2000.00	4.96804	9936.078	8454.857	46.464938	82993.798	84475.018	8454.857	84475.018
3000.00	4.96804	14904.117	13422.896	48.479304	130533.796	132015.017	13422.896	132015.017
4000.00	4.96804	19872.156	18390.935	49.908520	179761.924	181243.145	18390.935	181243.145
5000.00	4.96804	24840.195	23358.974	51.017106	230245.334	231726.555	23358.974	231726.555
6000.00	4.96804	29808.234	28327.013	51.922886	281729.085	283210.306	28327.013	283210.306
7000.00	4.95798	34781.304	33300.083	52.689521	334045.342	335526.563	33300.083	335526.563
8000.00	4.93560	39724.382	38243.161	53.349611	387072.505	388553.726	38243.161	388553.726
9000.00	4.95062	44665.471	43184.250	53.931569	440718.654	442199.875	43184.250	442199.875
10000.00	4.97741	49629.240	48148.019	54.454530	494916.059	496397.280	48148.019	496397.280
11000.00	5.00982	54621.832	53140.612	54.930351	549612.024	551093.244	53140.612	551093.244
12000.00	5.06987	59657.911	58176.690	55.368509	604764.201	606245.422	58176.690	606245.422
13000.00	5.19593	64783.554	63302.333	55.778713	660339.713	661820.934	63302.333	661820.934
14000.00	5.42838	70085.356	68604.135	56 171513	716315.821	717797.042	68604.135	717797.042
15000.00	5.79708	75685.955	74204.734	56.557768	772680.565	774161.786	74204.734	774161.786
16000.00	6.31165	81728.448	80247.227	56.947563	829432.560	830913.781	80247.227	830913.781
17000.00	6.95399	88352.220	86870.999	57.348930	886579.586	888060.807	86870.999	888060.807
18000.00	7.67267	95662.295	94181.074	57.766566	944135.893	945617.114	94181.074	945617.114
19000.00	8.37872	103693.801	102212.580	58.200635	1002118.258	1003599.479	102212.580	1003599.479
20000.00	8.94243	112372.762	110891.541	58.645683	1060540.895	1062022.116	110891.541	1062022.116

COEFFICIENTS BAR Argon

Example 2 (C_2H_3(g) by Method ADD with Wilhoit Extrapolation)

Problem.—Estimate thermodynamic properties for the C_2H_3 radical by adding group properties using method ADD and then extrapolate these properties to higher temperatures by means of the Wilhoit fit. Finally, obtain a least-squares fit of the previously generated data. C_2H_3 can be represented as being formed from two CDH2 groups $\left(\begin{array}{c} H \\ | \\ H-C= \end{array}\right)$ with a hydrogen atom removed by subtracting an HVIN group (See table IX). Inasmuch as the group data extend to only 3000 K, extrapolation to higher temperatures, e.g., to 5000 K, can be accomplished by means of the Wilhoit fit.

The input data set for example 2 consists of 12 records. The first is a NAME record giving the species name and comments. The second is a formula record. It gives a formula only. With method ADD, the heat of formation comes from the group additivity calculation and any value on the formula record is ignored. The DATE record gives a code (G 3/91) to represent Group additivity, March 1991. The OUTP record calls for a many-figured table (MFIG) in SI units (JOULES) and least-squares coefficients (LSQS). There are also two LSTS records giving five EXP values (q_i in eq. (11)) for the first temperature interval (1 in column 80), namely the default interval 298.15 to 1000 K. These are the same exponents as in the equation representing the group data (see table X). Since no information is given for the second interval, it will be the default interval of 1000 to 6000 K and the default equation for C_p^o with q_i values in equation (17).

There are two METH records each preceded by a set of corresponding TEMP records. For METH ADD, the temperature schedule is 298.15 K and 300 to 3000 K in 100-degree increments. For METH WILH, the schedule is 3500 to 6000 K in 500-degree increments. METH ADD is followed by one data record and METH WILH is the only method with no data records. The data record following the METH ADD record has a blank record ID. The labels on this record contain the group names, left-adjusted, followed by the number of times the group should be added or subtracted as well as the symmetry number (SYMNO) and statistical weight (STATWT) of the species formed. In this case all the numerical values are integers which should always be followed by a decimal. Numerical values should never encroach on the label spaces. The last record is the required FINISH record.

The first part of the output consists of input record images and some additional intermediate information. The molecular weight is inserted after the METH ADD record and the Wilhoit coefficients and integration constants are inserted after the METH WILH record image. The least-squares output is detailed in the section **Tables of least-squares errors**. The output table in SI units is described in appendix C in the section **Tables of original thermodynamic properties**. The columns for H-H0 and −(G-H0) are blank because no $H^o_{298.15} - H^o_0$ value (H298H0) was available.

Input. - The input data set for C_2H_3, example 2, is as follows:

	Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	C2H3 RADICAL		GROUP	ADDITION WITH WILHOIT EXTRAPOL			ATION.	Expl.	2
	C2H3									
	DATE	G 3/91								
	TEMP	T	298.15	T	300.	I	100.	T	3000.	
	OUTP	MFIG		JOULES		LSQS				
	LSTS	EXP	0.	EXP	1.	EXP	2.	EXP	3.	1
	LSTS	EXP	4.							1
	METH	ADD								
		CDH2	2.	HVIN	-1.	SYMNO	1.	STATWT	2.	
	TEMP	T	3500.	I	500.	T	6000.			
	METH	WILH								
	FINISH									

[a]All alphanumeric characters.

Listed output. - The listed output for C_2H_3, example 2, is as follows:

```
NAME  C2H3 RADICAL      GROUP ADDITION WITH WILHOIT EXTRAPOLATION.      Expl. 2
C2H3
DATE  G 3/91
OUTP  MFIG              JOULES            LSQS
LSTS  EXP      0.       EXP       1.      EXP      2.       EXP      3.        1
LSTS  EXP      4.                                                             1
TEMP  T      298.15     T      300.       I      100.      T      3000.
METH  ADD
MOLECULAR WT.=  27.04582
      CDH2      2.000000HVIN     -1.000000SYMNO     1.000000STATWT    2.000000
TEMP  T       3500.     I      500.       T       6000.
METH  WILH
   WILHOIT COEFFICIENTS
   A(0) =  0.924838250e+02     A(1) = -0.367448984e+03     A(2)          =  0.498539437e+03     A(3) = -0.225971567e+03
INTEGRATION CONSTANTS:     H/R = 0.788004609e+05     S/R =-0.172647715e+02
B =  150.0     CPO/R =   4.0000     CPI/R =  13.0000     NON-LINEAR     NO. ATOMS =   5

FINISH


LEAST SQUARES

      T      CP/R INPUT     CP/R CALC      HH/RT INPUT     HH/RT CALC      S/R INPUT      S/R CALC      -GH/RT INPUT     -GH/RT CALC
             INPUT-CALC      FRACTION       INPUT-CALC      FRACTION       INPUT-CALC      FRACTION       INPUT-CALC      FRACTION
    298.15    5.1334587     5.1334587      0.0000000     0.0000000     28.1531124     28.1531124     28.1531124     28.1531124
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    300.00    5.1531178     5.1531178      0.0317170     0.0317170     28.1849275     28.1849275     28.1532105     28.1532105
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    400.00    6.1157304     6.1157304      1.4362780     1.4362780     29.8036844     29.8036844     28.3674064     28.3674064
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    500.00    6.9177687     6.9177687      2.4546466     2.4546466     31.2570661     31.2570661     28.8024195     28.8024195
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    600.00    7.6026413     7.6026413      3.2569567     3.2569567     32.5803752     32.5803752     29.3234185     29.3234185
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    700.00    8.2006088     8.2006088      3.9213848     3.9213848     33.7982078     33.7982078     29.8768230     29.8768230
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    800.00    8.7287846     8.7287846      4.4899800     4.4899800     34.9284533     34.9284533     30.4384733     30.4384733
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
    900.00    9.1911343     9.1911343      4.9872741     4.9872741     35.9839172     35.9839172     30.9966431     30.9966431
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
   1000.00    9.5784758     9.5784758      5.4277252     5.4277252     36.9730816     36.9730816     31.5453565     31.5453565
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
 MAX REL ERR CP/R  =  0.000000    TEMP =   400.     AVER REL ERR CP/R  =  0.000000     REL LST SQ ERR CP/R  =  0.000000
 MAX REL ERR HH/RT =  0.000000    TEMP =   400.     AVER REL ERR HH/RT =  0.000000     REL LST SQ ERR HH/RT =  0.000000
 MAX REL ERR S/R   =  0.000000    TEMP =   500.     AVER REL ERR S/R   =  0.000000     REL LST SQ ERR S/R   =  0.000000
 MAX REL ERR GH/RT =  0.000000    TEMP =   700.     AVER REL ERR GH/RT =  0.000000     REL LST SQ ERR GH/RT =  0.000000
     MAX ERR CP/R  =  0.000000    TEMP.=   900.        AVER ERR CP/R  =  0.000000          LST SQ ERR CP/R  =  0.000000
     MAX ERR HH/RT =  0.000000    TEMP =   500.        AVER ERR HH/RT =  0.000000          LST SQ ERR HH/RT =  0.000000
     MAX ERR S/R   =  0.000000    TEMP =   500.        AVER ERR S/R   =  0.000000          LST SQ ERR S/R   =  0.000000
     MAX ERR GH/RT =  0.000000    TEMP =   700.        AVER ERR GH/RT =  0.000000          LST SQ ERR GH/RT =  0.000000
CP/R =    6.7053736e-01T** 0.0   2.0520078e-02T** 1.0  -2.3229402e-05T** 2.0   1.7095426e-08T** 3.0  -5.4781628e-12T** 4.0

(H-HO)/R CONSTANT = -0.93794084e+03, H/R CONSTANT = 0.80540638e+05, S/R CONSTANT = 0.19106863e+02

      T      CP/R INPUT     CP/R CALC      HH/RT INPUT     HH/RT CALC      S/R INPUT      S/R CALC      -GH/RT INPUT     -GH/RT CALC
             INPUT-CALC      FRACTION       INPUT-CALC      FRACTION       INPUT-CALC      FRACTION       INPUT-CALC      FRACTION
   1000.00    9.5784758     9.5784758      5.4277252     5.4277252     36.9730816     36.9730816     31.5453565     31.5453565
              0.0000000     0.0000000      0.0000000     0.0000000      0.0000000      0.0000000      0.0000000      0.0000000
   1100.00    9.9445347     9.9476608      5.8221381     5.8222637     37.9036300     37.9037585     32.0814919     32.0814948
             -0.0031261    -0.0003144     -0.0001256    -0.0000216     -0.0001285     -0.0000034     -0.0000029     -0.0000001
   1200.00   10.2624975    10.2657416      6.1792256     6.1796283     38.7828698     38.7832985     32.6036442     32.6036702
             -0.0032441    -0.0003161     -0.0004027    -0.0000652     -0.0004287     -0.0000111     -0.0000260     -0.0000008
   1300.00   10.5390577    10.5402211      6.5042090     6.5047584     39.6154873     39.6161020     33.1112782     33.1113436
             -0.0011634    -0.0001104     -0.0005493    -0.0000845     -0.0006147     -0.0000155     -0.0000653     -0.0000029
   1400.00   10.7792887    10.7778462      6.8011941     6.8016934     40.4055165     40.4061212     33.6043224     33.6044273
              0.0014425     0.0001338     -0.0004994    -0.0000734     -0.0006047     -0.0000150     -0.0001054     -0.0000031
   1500.00   10.9878845    10.9844061      7.0735169     7.0738138     41.1564927     41.1569231     34.0829758     34.0831093
              0.0034784     0.0003166     -0.0002968    -0.0000420     -0.0004304     -0.0000105     -0.0001336     -0.0000039
   1600.00   11.1691592    11.1647661      7.3239614     7.3239872     41.8715572     41.8717272     34.5475958     34.5477400
              0.0043931     0.0003933     -0.0000258    -0.0000035     -0.0001700     -0.0000041     -0.0001442     -0.0000042
   1700.00   11.3270474    11.3229793      7.5548989     7.5546685     42.5535297     42.5534371     34.9986308     34.9987686
              0.0040681     0.0003592      0.0002304     0.0000305      0.0000926      0.0000022     -0.0001378     -0.0000039
   1800.00   11.4651042    11.4624113      7.7683818     7.7679722     43.2049603     43.2046699     35.4365785     35.4366973
              0.0026928     0.0002349      0.0004095     0.0000527      0.0002904      0.0000067     -0.0001191     -0.0000034
   1900.00   11.5865047    11.5858573      7.9662075     7.9657297     43.8281674     43.8277842     35.8619599     35.8620545
              0.0006474     0.0000559      0.0004778     0.0000600      0.0003832      0.0000087     -0.0000946     -0.0000026
   2000.00   11.6940448    11.6956421      8.1499633     8.1495333     44.4252656     44.4249065     36.2753024     36.2753732
             -0.0015973    -0.0001366      0.0004300     0.0000528      0.0003591      0.0000081     -0.0000708     -0.0000020
   2100.00   11.7901404    11.7937042      8.3210581     8.3207735     44.9981873     44.9979557     36.6771292     36.6771822
             -0.0035638    -0.0003023      0.0002846     0.0000342      0.0002316      0.0000051     -0.0000530     -0.0000014
   2200.00   11.8768279    11.8816646      8.4807461     8.4806866     45.5486655     45.5486655     37.0679524     37.0679969
             -0.0048367    -0.0004072      0.0000775     0.0000091      0.0000331      0.0000007     -0.0000444     -0.0000012
   2300.00   11.9557641    11.9608826      8.6301433     8.6302896     46.0784120     46.0786042     37.4482686     37.4483146
             -0.0051185    -0.0004281     -0.0001463    -0.0000169     -0.0001922     -0.0000042     -0.0000459     -0.0000012
   2400.00   12.0282262    12.0325018      8.7702412     8.7705810     46.5887969     46.5891931     37.8185557     37.8186121
             -0.0042756    -0.0003555     -0.0003398    -0.0000387     -0.0003962     -0.0000085     -0.0000564     -0.0000015
   2500.00   12.0951116    12.0974869      8.9019158     8.9023782     47.0811868     47.0817223     38.1792710     38.1793441
             -0.0023753    -0.0001964     -0.0004624    -0.0000519     -0.0005355     -0.0000114     -0.0000731     -0.0000019
   2600.00   12.1569382    12.1566540      9.0259358     9.0264223     47.5567863     47.5573649     38.5308506     38.5309426
              0.0002843     0.0000234     -0.0004865    -0.0000539     -0.0005786     -0.0000122     -0.0000921     -0.0000024
   2700.00   12.2138442    12.2106952      9.1429680     9.1433724     48.0166759     48.0171895     38.8737079     38.8738171
              0.0031490     0.0002578     -0.0004045    -0.0000442     -0.0005136     -0.0000107     -0.0001092     -0.0000028
   2800.00   12.2655882    12.2601994      9.2535822     9.2538164     48.4618162     48.4621714     39.2082340     39.2083550
              0.0053888     0.0004393     -0.0002342    -0.0000253     -0.0003552     -0.0000073     -0.0001210     -0.0000031
   2900.00   12.3115491    12.3056685      9.3582548     9.3582797     48.8930517     48.8932022     39.5347970     39.5349226
              0.0058806     0.0004777     -0.0000249    -0.0000027     -0.0001505     -0.0000031     -0.0001256     -0.0000032
   3000.00   12.3507263    12.3475319      9.4573714     9.4572332     49.3111136     49.3110987     39.8537625     39.8538656
              0.0031944     0.0002586      0.0001383     0.0000146      0.0000149      0.0000003     -0.0001234     -0.0000031

              ORIGINÁL          BAR    C2H3 RADICAL
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3500.00	12.5136171	12.5139980	9.8830643	9.8827806	51.2279962	51.2277975	41.3449320	41.3450169
	-0.0003809	-0.0000304	0.0002836	0.0000287	0.0001987	0.0000039	-0.0000849	-0.0000021
4000.00	12.6258090	12.6286924	10.2193107	10.2192865	52.9067248	52.9067615	42.6874141	42.6874750
	-0.0028834	-0.0002284	0.0000242	0.0000024	-0.0000368	-0.0000007	-0.0000609	-0.0000014
4500.00	12.7057216	12.7082897	10.4913770	10.4916897	54.3986970	54.3990884	43.9073201	43.9073987
	-0.0025681	-0.0002021	-0.0003127	-0.0000298	-0.0003914	-0.0000072	-0.0000787	-0.0000018
5000.00	12.7644316	12.7638239	10.7158907	10.7162859	55.7405685	55.7410827	45.0246778	45.0247963
	0.0006078	0.0000476	-0.0003952	-0.0000369	-0.0005142	-0.0000092	-0.0001190	-0.0000026
5500.00	12.8086825	12.8053269	10.9042239	10.9043782	56.9593193	56.9596208	46.0550954	46.0552426
	0.0033555	0.0002620	-0.0001544	-0.0000142	-0.0003015	-0.0000053	-0.0001472	-0.0000032
6000.00	12.8427587	12.8442720	11.0644080	11.0643857	58.0753434	58.0754710	47.0109354	47.0110853
	-0.0015133	-0.0001178	0.0000223	0.0000020	-0.0001276	-0.0000022	-0.0001499	-0.0000032

MAX REL ERR CP/R	= 0.000478	TEMP = 2900.	AVER REL ERR CP/R	= 0.000237	REL LST SQ ERR CP/R	= 0.000274
MAX REL ERR HH/RT	= 0.000084	TEMP = 1300.	AVER REL ERR HH/RT	= 0.000033	REL LST SQ ERR HH/RT	= 0.000040
MAX REL ERR S/R	= 0.000016	TEMP = 1300.	AVER REL ERR S/R	= 0.000007	REL LST SQ ERR S/R	= 0.000008
MAX REL ERR GH/RT	= 0.000004	TEMP = 1600.	AVER REL ERR GH/RT	= 0.000002	REL LST SQ ERR GH/RT	= 0.000003
MAX ERR CP/R	= 0.005881	TEMP = 2900.	AVER ERR CP/R	= 0.002786	LST SQ ERR CP/R	= 0.003226
MAX ERR HH/RT	= 0.000549	TEMP = 1300.	AVER ERR HH/RT	= 0.000268	LST SQ ERR HH/RT	= 0.000318
MAX ERR S/R	= 0.000615	TEMP = 1300.	AVER ERR S/R	= 0.000299	LST SQ ERR S/R	= 0.000354
MAX ERR GH/RT	= 0.000150	TEMP = 6000.	AVER ERR GH/RT	= 0.000088	LST SQ ERR GH/RT	= 0.000098

CP/R = 2 0575702e+06T**-2.0 -9.4600005e+03T**-1.0 1.8762547e+01T** 0.0 -2.2520423e-03T** 1.0 5.3448381e-07T** 2.0
-6.7520919e-11T** 3.0 3.4387285e-15T** 4.0
(H-H0)/R CONSTANT = 0.55034170e+05, H/R CONSTANT = 0.13651275e+06, S/R CONSTANT =-0.99058768e+02

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

```
C2H3 RADICAL      GROUP ADDITION WITH WILHOIT EXTRAPOLATION.       Expl, 2
 2 G 3/91 C    2.00H    3.00     0.00     0.00     0.00 0     27.04582     677454.462
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0              0.000
  6.70537360d-01  2.05200777d-02 -2.32294021d-05  1.70954257d-08 -5.47816280d-12
  0.00000000d+00  0.00000000d+00  0.00000000d+00  8.05406384d+04  1.91068625d+01
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0              0.000
  2.05757019d+06 -9.46000054d+03  1.87625468d+01 -2.25204228d-03  5.34483811d-07
 -6.75209185d-11  3.43872846d-15  0.00000000d+00  1.36512749d+05 -9.90587681d+01
```

ORIGINAL C2H3 RADICAL

ASSIGNED H AT 298 K = 677454.462 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
298.15	42.68219		0.000	234.079335		69790.754	677454.462	-607663.708
300.00	42.84565		79.113	234.343862		70224.045	677533.575	-607230.417
400.00	50.84930		4776.779	247.803032		94344.434	682231.241	-583110.028
500.00	57.51786		10204.592	259.887189		119739.002	687659.054	-557715.459
600.00	63.21224		16247.999	270.889856		146285.914	693702.461	-531168.548
700.00	68.18404		22823.075	281.015536		173887.801	700277.537	-503566.661
800.00	72.57557		29865.587	290.412974		202464.793	707320.049	-474989.669
900.00	76.41978		37320.066	299.188639		231949.709	714774.528	-445504.753
1000.00	79.64033		45128.875	307.413057		262284.182	722583.337	-415170.230
1100.00	82.68393		53249.048	315.150111		293416.074	730703.510	-384038.388
1200.00	85.32764		61652.679	322.460558		325299.991	739107.141	-352154.471
1300.00	87.62710		70303.105	329.383365		357895.270	747757.566	-319559.192
1400.00	89.62450		79168.034	335.952071		391164.865	756622.496	-286289.597
1500.00	91.35888		88219.241	342.196070		425074.864	765673.703	-252379.597
1600.00	92.86609		97432.241	348.141481		459594.129	774886.703	-217860.333
1700.00	94.17885		106785.980	353.811748		494693.992	784240.442	-182760.470
1800.00	95.32672		116262.518	359.228074		530348.016	793716.980	-147106.446
1900.00	96.33611		125846.712	364.409736		566531.786	803301.174	-110922.676
2000.00	97.23025		135525.902	369.374315		603222.729	812980.364	-74231.733
2100.00	98.02924		145289.594	374.137878		640399.950	822744.056	-37054.512
2200.00	98.75000		155129.146	378.715109		678044.095	832583.608	589.633
2300.00	99.40632		165037.450	383.119417		716137.209	842491.912	38682.748
2400.00	100.00881		175008.619	387.363017		754662.623	852463.081	77208.161
2500.00	100.56493		185037.670	391.456999		793604.827	862492.132	116150.365
2600.00	101.07898		195120.206	395.411375		832949.370	872574.668	155494.908
2700.00	101.55213		205252.106	399.235132		872682.749	882706.568	195228.237
2800.00	101.98236		215429.205	402.936255		912792.310	892883.667	235337.848
2900.00	102.36450		225646.978	406.521767		953266.147	903101.440	275811.686
3000.00	102.69024		235900.228	409.997747		994093.013	913354.690	316638.551
3500.00	104.04459		287604.928	425.935687		1203169.977	965059.390	525715.515
4000.00	104.97742		339874.244	439.893492		1419699.725	1017328.706	742245.263
4500.00	105.64185		392537.964	452.298511		1642805.334	1069992.426	965350.872
5000.00	106.12999		445486.902	463.455514		1871790.669	1122941.364	1194336.208
5500.00	106.49792		498648.031	473.588830		2106090.531	1176102.493	1428636.070
6000.00	106.78125		551970.787	482.868024		2345237.356	1229425.249	1667782.894

ORIGINAL BAR C2H3 RADICAL

Example 3 (C_4H_4(g) by Method READIN with Wilhoit Extrapolation)

Problem.—Use method READIN to process thermodynamic data obtained from the literature. Inasmuch as the data to be processed are available to only 1500 K, use the Wilhoit fit to extrapolate to higher temperatures.

The input follows the same pattern as in the first two examples. The NAME record gives the name and reference for the species. The second record, the required formula record, gives the formula and heat of formation at 298.15 K (HF298)—namely, 435 000 J/mol. This is followed by a DATE record where X10/85 was chosen to represent the Texas TRC Thermodynamic Tables along with the date of the particular table. The two REFN records give more information on the reference. The first label ATM on the OUTP record specifies that the pressure unit in the output entropy and Gibbs energy functions be in atmospheres rather than the default unit which is bars. The remaining OUTP record labels call for many figures tables (MFIG), in both dimensionless (DMLESS) and joules (JOULES) energy units.

There are two METH records. The first is a READIN method with no preceding TEMP records since the temperatures for the data come from the data records. The METH WILH record is for Wilhoit extrapolation and the TEMP record which precedes it gives the extrapolation schedule. The KJOULE label on the METH READIN record specifies that the input enthalpy values are in units of kJ/mol. However, C_p^o and S_T^o values are in J/mol-K whether the label is KJOULE or JOULES. The BAR label specifies that the standard state pressure in the entropy values on the data records is one bar. The 19 data records have the optional record ID of C4H4. The METH WILH record has no other labels since the molecule is nonlinear, the default structure. Linear molecules require a LINE label. Since this method has no data records, it is followed by the final FINISH record.

The listed output consists of the input record images, the Wilhoit coefficients and integration constants, and the two tables requested on the OUTP record. It should be noted that the OUTP record specifies one atmosphere (ATM) for the output standard state entropy pressure while the METH record indicates the standard state pressure is one bar (BAR) for the input entropy. Thus, at $T = 298.15$ K, $S_T^o = 251.67$ J/mol-K in the input and $S_T^o = 251.56$ J/mol-K in the output.

Input. - The input data set for C_4H_4, example 3, is as follows:

	Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	CYCLOBUTADIENE		TRC TABLES T,U,V,W	-2920,	OCT 31, 1985.		Expl.		3
	C4H4			HF298	435000.	JOULES				
	DATE	X10/85								
a	REFN	TRC THERMODYNAMIC		TABLES - HYDROCARBONS.		The Texas A&M University System,				
a	REFN	College Station,		TX 77843-3111.		Tables t,u,v,w-2920, Oct.31,1985.				
	OUTP	ATM		DMLESS		MFIG		JOULES		
	METH	READIN		KJOULE		BAR				
	C4H4	T	50.000	CP	33.2600	H-H0	0.166300D 01	S	182.78000	
	C4H4	T	100.000	CP	33.6300	H-H0	0.333000D 01	S	205.88000	
	C4H4	T	150.000	CP	36.6100	H-H0	0.507100D 01	S	219.96000	
	C4H4	T	200.000	CP	43.0200	H-H0	0.705000D 01	S	231.30000	
	C4H4	T	273.160	CP	55.9800	H-H0	0.106550D 02	S	246.56000	
	C4H4	T	298.150	CP	60.7500	H-H0	0.121140D 02	S	251.67000	
	C4H4	T	300.000	CP	61.1000	H-H0	0.122270D 02	S	252.04000	
	C4H4	T	400.000	CP	79.3000	H-H0	0.192670D 02	S	272.17000	
	C4H4	T	500.000	CP	94.4500	H-H0	0.279830D 02	S	291.56000	
	C4H4	T	600.000	CP	106.5000	H-H0	0.380530D 02	S	309.88000	
	C4H4	T	700.000	CP	116.1700	H-H0	0.492040D 02	S	327.05000	
	C4H4	T	800.000	CP	124.1200	H-H0	0.612310D 02	S	343.10000	
	C4H4	T	900.000	CP	130.8100	H-H0	0.739900D 02	S	358.12000	
	C4H4	T	1000.000	CP	136.5000	H-H0	0.873600D 02	S	372.20000	
	C4H4	T	1100.000	CP	141.5000	H-H0	0.101260D 03	S	385.50000	
	C4H4	T	1200.000	CP	145.7000	H-H0	0.115630D 03	S	398.00000	
	C4H4	T	1300.000	CP	149.4000	H-H0	0.130390D 03	S	409.80000	
	C4H4	T	1400.000	CP	152.7000	H-H0	0.145500D 03	S	421.00000	
	C4H4	T	1500.000	CP	155.5000	H-H0	0.160920D 03	S	431.60000	
	TEMP	T	1600.	I	200.	T	5000.			
	METH	WILH								
	FINISH									

[a]All alphanumeric characters.

Listed output. - The listed output for C_4H_4, example 3, is as follows:

```
NAME  CYCLOBUTADIENE    TRC TABLES T,U,V,W-2920, OCT 31, 1985.          Expl. 3
C4H4                    HF298   435000.   JOULES
DATE  X10/85
REFN  TRC THERMODYNAMIC TABLES - HYDROCARBONS.  The Texas A&M University System,
REFN    College Station, TX 77843-3111.  Tables t,u,v,w-2920, Oct.31,1985.
OUTP  ATM               DMLESS            MFIG              JOULES
METH  READIN            KJOULE            BAR
C4H4  T         50.000  CP       33.2600  H-H0  0.166300D 01S        182.78000
C4H4  T        100.000  CP       33.6300  H-H0  0.333000D 01S        205.88000
C4H4  T        150.000  CP       36.6100  H-H0  0.507100D 01S        219.96000
C4H4  T        200.000  CP       43.0200  H-H0  0.705000D 01S        231.30000
C4H4  T        273.160  CP       55.9800  H-H0  0.106550D 02S        246.56000
C4H4  T        298.150  CP       60.7500  H-H0  0.121140D 02S        251.67000
C4H4  T        300.000  CP       61.1000  H-H0  0.122270D 02S        252.04000
C4H4  T        400.000  CP       79.3000  H-H0  0.192670D 02S        272.17000
C4H4  T        500.000  CP       94.4500  H-H0  0.279830D 02S        291.56000
C4H4  T        600.000  CP      106.5000  H-H0  0.380530D 02S        309.88000
C4H4  T        700.000  CP      116.1700  H-H0  0.492040D 02S        327.05000
C4H4  T        800.000  CP      124.1200  H-H0  0.612310D 02S        343.10000
C4H4  T        900.000  CP      130.8100  H-H0  0.739900D 02S        358.12000
C4H4  T       1000.000  CP      136.5000  H-H0  0.873600D 02S        372.20000
C4H4  T       1100.000  CP      141.5000  H-H0  0.101260D 03S        385.50000
C4H4  T       1200.000  CP      145.7000  H-H0  0.115630D 03S        398.00000
C4H4  T       1300.000  CP      149.4000  H-H0  0.130390D 03S        409.80000
C4H4  T       1400.000  CP      152.7000  H-H0  0.145500D 03S        421.00000
C4H4  T       1500.000  CP      155.5000  H-H0  0.160920D 03S        431.60000
                                ATM    CYCLOBUTADIENE


TEMP  T      1600.      I       200.      T       5000.
METH  WILH
   WILHOIT COEFFICIENTS
   A(0) =  0.415261964e+00     A(1) =  0.540942637e+01     A(2)         = -0.610546449e+01     A(3) = -0.117525765e+01
INTEGRATION CONSTANTS:     H/R = 0.103765248e+05     S/R =-0.890756216e+02
B =  200.0     CPO/R =   4.0000     CPI/R =  22.0000     NON-LINEAR     NO. ATOMS =   8

FINISH


                ORIGINAL          ATM    CYCLOBUTADIENE
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ORIGINAL CYCLOBUTADIENE

ASSIGNED H/R AT 0 K = 50861.205 K

T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
50.00	4.00024	4.0002357	-25.1391844	21.9700928	17.9698570	47.1092772	1021.2243415	-999.2542488
100.00	4.04474	4.0050466	-10.5646635	24.7483683	20.7433217	35.3130318	512.6170995	-487.8687312
150.00	4.40315	4.0659842	-5.6471558	26.4417935	22.3758092	32.0889493	343.1406862	-316.6988927
200.00	5.17409	4.2395764	-3.0452787	27.8056742	23.5660978	30.8509529	258.5456028	-230.7399286
273.16	6.73281	4.6913700	-0.6423941	29.6410199	24.9496498	30.2834139	190.8870257	-161.2460058
298.15	7.30650	4.8867047	0.0000000	30.2556081	25.3689034	30.2556081	175.4760231	-145.2204150
300.00	7.34860	4.9018723	0.0453023	30.3001086	25.3982363	30.2548063	174.4392233	-144.1391147
400.00	9.53754	5.7931856	2.1507581	32.7211773	26.9279917	30.5704192	132.9461989	-100.2250215
500.00	11.35966	6.7311243	3.8171823	35.0532450	28.3221207	31.2360628	108.4535348	-73.4002898
600.00	12.80893	7.6278297	5.1995447	37.2566220	29.6287922	32.0570773	92.3965052	-55.1398832
700.00	13.97196	8.4540675	6.3726803	39.3216866	30.8676191	32.9490062	81.1129322	-41.7912456
800.00	14.92812	9.2054433	7.3842295	41.2520469	32.0466036	33.8678174	72.7819499	-31.5299030
900.00	15.73274	9.8876676	8.2688109	43.0585273	33.1708597	34.7897164	66.4001179	-23.3415906
1000.00	16.41708	10.5069331	9.0499621	44.7519524	34.2450194	35.7019904	61.3681384	-16.6161859
1100.00	17.01844	11.0715539	9.7470348	46.3515656	35.2800118	36.6045309	57.3090132	-10.9574476
1200.00	17.52358	11.5891776	10.3750351	47.8549615	36.2657839	37.4799264	53.9735154	-6.1185539
1300.00	17.96859	12.0632485	10.9425015	49.2741672	37.2109188	38.3316657	51.1872525	-1.9130853
1400.00	18.36548	12.4996628	11.4589692	50.6212099	38.1215471	39.1622407	48.8290952	1.7921148
1500.00	18.70224	12.9027447	11.9314307	51.8960896	38.9933449	39.9646589	46.8102149	5.0858747
1600.00	18.89517	13.2691069	12.3585000	53.1070325	39.8379256	40.7485325	45.0573602	8.0496723
1800.00	19.33589	13.9197380	13.1103097	55.3590988	41.4393608	42.2487891	42.1759632	13.1831356
2000.00	19.68191	14.4793212	13.7508357	57.4149494	42.9356282	43.6641137	39.9099238	17.5050256
2200.00	19.95893	14.9653234	14.3030638	59.3042970	44.3389736	45.0012332	38.0840530	21.2202440
2400.00	20.18447	15.3911641	14.7840929	61.0509441	45.6597799	46.2668512	36.5833330	24.4676111
2600.00	20.37080	15.7672659	15.2068925	62.6741498	46.9068838	47.4672573	35.3292680	27.3448818
2800.00	20.52673	16.1018181	15.5814713	64.1896603	48.0878422	48.6081890	34.2665343	29.9231260
3000.00	20.65870	16.4013296	15.9156726	65.6104809	49.2091514	49.6948084	33.3550647	32.2554163
3200.00	20.77154	16.6710308	16.2157274	66.9474573	50.2764264	50.7317299	32.5651575	34.3822998
3400.00	20.86888	16.9151685	16.4866476	68.2097152	51.2945467	51.7230676	31.8743465	36.3353637
3600.00	20.95353	17.1372236	16.7325095	69.4049981	52.2677745	52.6724887	31.2653362	38.1396619
3800.00	21.02769	17.3400752	16.9566618	70.5399269	53.1998517	53.5832651	30.7246029	39.8153240
4000.00	21.09308	17.5261239	17.1618812	71.6202032	54.0940793	54.4583220	30.2414252	41.3787780
4200.00	21.15109	17.6973870	17.3504892	72.6507692	54.9533822	55.3002801	29.8071978	42.8435714
4400.00	21.20284	17.8555715	17.5244417	73.6359350	55.7803635	56.1114933	29.4149364	44.2209986
4600.00	21.24923	18.0021314	17.6853986	74.5794805	56.5773490	56.8940819	29.0589152	45.5205653
4800.00	21.29102	18.1383128	17.8347772	75.4847378	57.3464250	57.6499606	28.7343973	46.7503405
5000.00	21.32882	18.2651896	17.9737954	76.3546587	58.0894691	58.3808633	28.4374306	47.9172281

ORIGINAL ATM CYCLOBUTADIENE

ORIGINAL CYCLOBUTADIENE

ASSIGNED H AT 0 K = 422886.000 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
50.00	33.26000	1663.000	-10451.000	182.670556	7470.528	19584.528	424549.000	-415415.472
100.00	33.63000	3330.000	-8784.000	205.770556	17247.056	29361.056	426216.000	-405638.944
150.00	36.61000	5071.000	-7043.000	219.850556	27906.583	40020.583	427957.000	-394979.417
200.00	43.02000	7050.000	-5064.000	231.190556	39188.111	51302.111	429936.000	-383697.889
273.16	55.98000	10655.000	-1459.000	246.450556	56665.434	68779.434	433541.000	-366220.566
298.15	60.75000	12114.000	0.000	251.560556	62888.780	75002.780	435000.000	-359997.220
300.00	61.10000	12227.000	113.000	251.930556	63352.167	75466.167	435113.000	-359533.833
400.00	79.30000	19267.000	7153.000	272.060556	89557.222	101671.222	442153.000	-333328.778
500.00	94.45000	27983.000	15869.000	291.450556	117742.278	129856.278	450869.000	-305143.722
600.00	106.50000	38053.000	25939.000	309.770556	147809.334	159923.334	460939.000	-275076.666
700.00	116.17000	49204.000	37090.000	326.940556	179654.389	191768.389	472090.000	-243231.611
800.00	124.12000	61231.000	49117.000	342.990556	213161.445	225275.445	484117.000	-209724.555
900.00	130.81000	73990.000	61876.000	358.010556	248219.500	260333.500	496876.000	-174666.500
1000.00	136.50000	87360.000	75246.000	372.090556	284730.556	296844.556	510246.000	-138155.444
1100.00	141.50000	101260.000	89146.000	385.390556	322669.612	334783.612	524146.000	-100216.338
1200.00	145.70000	115630.000	103516.000	397.890556	361838.667	373952.667	538516.000	-61047.333
1300.00	149.40000	130390.000	118276.000	409.690556	402207.723	414321.723	553276.000	-20678.277
1400.00	152.70000	145500.000	133386.000	420.890556	443746.779	455860.779	568386.000	20860.779
1500.00	155.50000	160920.000	148806.000	431.490556	486315.834	498429.834	583806.000	63429.834
1600.00	157.10409	176521.795	164407.795	441.558953	529972.529	542086.529	599407.795	107086.529
1800.00	160.76845	208324.442	196210.442	460.283781	620186.363	632300.363	631210.442	197300.363
2000.00	163.64548	240776.921	228662.921	477.377171	713977.420	726091.420	663662.921	291091.420
2200.00	165.94873	273744.528	261630.528	493.086170	811045.047	823159.047	696630.528	388159.047
2400.00	167.82394	307127.971	295013.971	507.608685	911132.872	923246.872	730013.971	488246.872
2600.00	169.37318	340852.435	328738.435	521.104845	1014020.162	1026134.162	763738.435	591134.162
2800.00	170.66967	374860.437	362746.437	533.705572	1119515.165	1131629.165	797746.437	696629.165
3000.00	171.76700	409107.056	396993.056	545.519000	1227449.944	1239563.944	831993.056	804563.944
3200.00	172.70516	443556.648	431442.648	556.635303	1337676.322	1349790.322	866442.648	914790.322
3400.00	173.51449	478180.548	466066.548	567.130359	1450062.674	1462176.674	901066.548	1027176.674
3600.00	174.21832	512955.422	500841.422	577.068551	1564491.362	1576605.362	935841.422	1141605.362
3800.00	174.83490	547862.069	535748.069	586.504928	1680856.657	1692970.657	970748.069	1257970.657
4000.00	175.37861	582884.530	570770.530	595.486896	1799063.053	1811177.053	1005770.530	1376177.053
4200.00	175.86095	618009.425	605895.425	604.055547	1919023.872	1931137.872	1040895.425	1496137.872
4400.00	176.29122	653225.443	641111.443	612.246718	2040660.116	2052774.116	1076111.443	1617774.116
4600.00	176.67697	688522.949	676408.949	620.091836	2163899.498	2176013.498	1111408.949	1741013.498
4800.00	177.02442	723893.680	711779.680	627.618607	2288675.634	2300789.634	1146779.680	1865789.634
5000.00	177.33871	759330.507	747216.507	634.851573	2414927.359	2427041.359	1182216.507	1992041.359

ORIGINAL ATM CYCLOBUTADIENE

Example 4 (C_5H_{11}(g) by Method RRHO with Internal Rotation)

Problem.—Calculate thermodynamic properties for a species with internal rotation using the RRHO method.

The comments for this species will be mainly with respect to the method (METH RRHO) and the data records. The remaining records are similar to those discussed in the first three examples. The method RRHO is the rigid rotator-harmonic oscillator approximation. Please refer to tables II and VII for the required data. The tert-pentyl radical is a nonlinear molecule and thus has a total of 3N-6 fundamental frequencies (Vi(d_i)values) and internal rotors (INTROT value), where N is the number of atoms in the molecule. In this case the number is 3(16)-6 = 42, with 38 frequencies and four rotors. Fourteen unique frequencies are given on the data records with their multiplicities given in parentheses. The rigid rotator part requires either the moments of inertia (IA,IB,IC) or rotational constants (A0,B0,C0) for the nonlinear molecule.. For this example the individual moments of inertia in $(g)(cm)^2 \times 10^{39}$ have been multiplied together into one value of 8590. with the label IAIBIC.

The four internal rotors are specified by the label INTROT and its corresponding numerical value of 4.. (Note that the record ID on the data records are all blank, which is one of the permitted options.) The data records for the individual rotors are identified by the number in column 80. The third and fourth rotors for C_5H_{11} have identical parameters so they may be combined by using NROTOR = 2. on the data record for the third rotor. The barrier potential for the first rotor is V3 = 1254. cm^{-1}. Inasmuch as no potentials are specified for the other rotors, the program treats them as free rotors. The IB values for the rotors are the moments of inertia in $(g)(cm)^2 \times 10^{39}$ and the ROSYM values are the symmetry numbers for the rotors.

Input. - The input data set for C_5H_{11}, example 4, is as follows:

	Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	TERT-P	ENTYL RAD	WING T	SANG, J.AM.C	H.SOC.,	MAY 15,198	5, P28	72. Expl.	4
	C5H11			HF298	32600.	JOULES				
	DATE	L 5/87								
a	REFN	WING T	SANG, 'THE S	TABILI	TY OF ALKYL	RADICA	LS,' J. AM.	CHEM.	SOC.	
a	REFN	MAY 15	,1985, PP 28	72-288	0.					
	TEMP	T	100.	T	1000.	I	1000.	T	6000.	
	OUTP	MFIG		DMLESS		JOULES		CAL		
	METH	RRHO								
		V1(9)	2931.	V2(2)	2825.	V3(8)	1455.	V4(3)	1370.	
		V5	1279.	V6(2)	1252.	V7(2)	1189.	V8	1126.	
		V9(3)	992.	V10	733.	V11(2)	541.	V12	380.	
		V13(1)	200.	V14(2)	990.	STATWT	2.	IAIBIC	8590.	
		INTROT	4.							
		NEL	100.			NROTOR	1.			1
		ROSYM	3.	V3	1254.	IB	.48			1
		ROSYM	1.	NROTOR	1.	IB	2.1			2
		ROSYM	3.	NROTOR	2.	IB	.48			3
	FINISH									

[a]All alphanumeric characters.

Listed output. - Listed output for C_5H_{11}, example 4, is as follows:

```
NAME  TERT-PENTYL RAD   WING TSANG, J.AM.CH.SOC., MAY 15,1985, P2872.    Expl. 4
C5H11                  HF298    32600.   JOULES
DATE  L 5/87
REFN  WING TSANG, 'THE STABILITY OF ALKYL RADICALS,' J. AM. CHEM. SOC.
REFN  MAY 15,1985, PP 2872-2880.
TEMP  T       100.     T      1000.      I      1000.      T      6000.
OUTP  MFIG             DMLESS            JOULES            CAL
METH  RRHO
MOLECULAR WT.=  71.14234
      V1(9)   2931.     V2(2)   2825.     V3(8)   1455.     V4(3)   1370.
      V5      1279.     V6(2)    1252.    V7(2)   1189.     V8      1126.
      V9(3)    992.     V10      733.     V11(2)  541.      V12     380.
      V13(1)   200.     V14(2)   990.     STATWT  2.        IAIBIC   8590.
      INTROT 4.
      NEL     100.                       NROTOR  1.                          1
      ROSYM   3.        V3      1254.    IB         .48                      1
      ROSYM   1.        NROTOR    1.     IB        2.1                       2
  MINIMUM OF POTENTIAL FUNCTION IS    0.000 CM**(-1)

  BARRIER POTENTIAL CONSTANTS IN CAL/MOL          0.00      0.00    3585.37      0.00      0.00      0.00
                          OR IN CM**(-1)         0.000     0.000   1254.000     0.000     0.000     0.000

  ROTATION CONSTANTS IN CM**(-1)                 5.83183   0.00000   0.00000   0.00000

      ROSYM   3.        NROTOR    2.     IB         .48                      3
  V=0 FOR ROTOR  2. USE CLASSICAL PARTITION FUNCTION FOR FREE ROTOR (IROTOR).
FINISH
  V=0 FOR ROTOR  3. USE CLASSICAL PARTITION FUNCTION FOR FREE ROTOR (IROTOR).
              ORIGINAL          BAR    TERT-PENTYL RAD
```

ORIGINAL TERT-PENTYL RAD

ASSIGNED H/R AT 0 K = 1558.273 K

T	CP/R	(H-H0)/RT	(H-H298)/RT	S/R	-(G-H0)/RT	-(G-H298)/RT	H/RT	-G/RT
100.00	6.60920	5.8128262	-17.8130086	34.7528978	28.9400716	52.5659063	21.3955557	13.3573420
298.15	11.88955	7.9241438	0.0000000	44.0766593	36.1525155	44.0766593	13.1506169	30.9260424
1000.00	30.82205	18.3487024	15.9861190	69.2977936	50.9490911	53.3116746	19.9069754	49.3908182
2000.00	39.26581	27.1681671	25.9868754	93.9084148	66.7402477	67.9215394	27.9473036	65.9611112
3000.00	41.70940	31.6782837	30.8907559	110.3772014	78.6989178	79.4864456	32.1977080	78.1794934
4000.00	42.67036	34.3221130	33.7314672	122.5262009	88.2040879	88.7947338	34.7116813	87.8145197
5000.00	43.13628	36.0433197	35.5708030	132.1034232	96.0601035	96.5326202	36.3549743	95.7484439
6000.00	43.39522	37.2489471	36.8551832	139.9930650	102.7441179	103.1378818	37.5086593	102.4844057

ORIGINAL TERT-PENTYL RAD

ASSIGNED H AT 0 K = 12956.276 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
100.00	54.95223	4833.080	-14810.644	288.953316	24062.251	43705.975	17789.356	11105.975
298.15	98.85578	19643.724	0.000	366.475825	89621.043	109264.767	32600.000	76664.767
1000.00	256.27026	152560.470	132916.746	576.177198	423616.728	443260.452	165516.746	410660.452
2000.00	326.47595	451779.994	432136.270	780.802454	1109824.913	1129468.637	464736.270	1096868.637
3000.00	346.79319	790168.220	770524.496	917.732345	1963028.816	1982672.540	803124.496	1950072.540
4000.00	354.78317	1141486.208	1121842.484	1018.745323	2933495.084	2953138.807	1154442.484	2920538.807
5000.00	358.65700	1498412.710	1478768.987	1098.375233	3993463.456	4013107.180	1511368.987	3980507.130
6000.00	360.80997	1858240.461	1838596.737	1163.973739	5125601.972	5145245.696	1871196.737	5112645.696

ORIGINAL TERT-PENTYL RAD

ASSIGNED H AT 0 K = 3096.624 CAL/MOLE

T DEG-K	CP CAL/MOL-K	H-H0 CAL/MOL	H-H298 CAL/MOL	S CAL/MOL-K	-(G-H0) CAL/MOL	-(G-H298) CAL/MOL	H CAL/MOL	-G CAL/MOL
100.00	13.13390	1155.134	-3539.829	69.061500	5751.016	10445.979	4251.758	2654.392
298.15	23.62710	4694.963	0.000	87.589824	21419.943	26114.906	7791.587	18323.319
1000.00	61.25006	36462.827	31767.865	137.709655	101246.828	105941.791	39559.452	98150.204
2000.00	78.02963	107978.010	103283.047	186.616265	265254.520	269949.483	111074.634	262157.896
3000.00	82.88556	188854.737	184159.774	219.343295	469175.147	473870.110	191951.361	466078.523
4000.00	84.79521	272821.751	268126.789	243.485976	701122.152	705817.115	275918.376	698025.528
5000.00	85.72108	358129.233	353434.270	262.517981	954460.673	959155.636	361225.857	951364.049
6000.00	86.23565	444130.129	439435.167	278.196400	1225048.273	1229743.235	447226.754	1221951.648

Example 5 (H_2O(g) by Method NRRAO2 with Intermediate Output)

Problem.—Calculate thermodynamic functions for H_2O(g) using method NRRAO2. List some intermediate results in addition to final tables.

This is the only one of the eight examples discussed which does not start with a NAME record. This optional record was intentionally omitted to show that, as a result, the output tables are not identified by species name on the bottom of the listings. Therefore, while the NAME record is optional, it is generally useful to include it.

A REFNCE record was used to indicate the example number. This is followed by the formula record. It gives the formula with all the stoichiometric coefficients and an assigned enthalpy (ASINDH) of −57103.5 cal/mol (CAL) at $T = 0$ K. The TEMP record indicates a temperature schedule of only one value, 5000 K. The OUTP record calls for intermediate output (INTERM) and a many-figured table (MFIG) in energy units of joules (JOULES).

The NRRAO1 and NRRAO2 methods are the only methods in PAC91 that can accommodate the large variety of spectroscopic constants available for H_2O(g). In addition to the fundamental frequencies ν_i and rotational constants A_0, B_0, and C_0, other constants included are the anharmonicities x_{ij} and y_{ijk}; vibration-rotation interaction constants α_i^A(ALFAAi), α_i^B(ALFABi), and α_i^C(ALFACi) for $i = 1$, 2 and 3; rotation-stretching constant ρ; and symmetry number (SYMNO). These spectroscopic constants appear on the nine data records following the METHOD NRRAO2 record. The FINISH record is last, as usual.

The intermediate output follows the input record images for each electronic state plus one record. For this case there is only the ground state and the intermediate output follows the FINISH record. This output is discussed in section **Intermediate data with INTERM label** in appendix C. The last item listed is the many-figured table with properties at 5000 K and energy units in joules.

Input. - The input data set for H_2O, example 5, is as follows:

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
REFNCE								Expl.	5
H2O1			ASINDH	-57103.5	CAL		T	0.	
TEMP	T	5000.							
OUTP	INTERM		MFIG		JOULES				
METHOD			NRRAO2						
DATA	V1	3656.65	V2	1594.78	V3	3755.79	X11	-45.18	
DATA	X12	-15.14	X33	-44.62	X13	-165.48	X22	-17.04	
DATA	Y233	-.81	Y333	-.45	X23	-19.99			
DATA	Y111	.47	Y112	-.10	Y113	.68	Y122	-0.1	
DATA	Y123	-1.72	Y133	1.17	Y222	-.60	Y223	1.55	
DATA	A0	27.848	B0	14.5064	C0	9.28285	SYMNO	2.	
DATA	ALFAA1	.750	ALFAA2	-2.941	ALFAA3	1.253	ALFAB1	.238	
DATA	ALFAB2	-.160	ALFAB3	.078	ALFAC1	.2018	ALFAC2	.1392	
DATA	ALFAC3	.1445	RHO	.0000213	STATWT	1.			
FINISH									

[a] All alphanumeric characters.

Listed output. - The listed output for H_2O, example 5, is as follows:

```
REFNCE                                                          Expl. 5
H2O1                    ASINDH -57103.5   CAL               T          0.
TEMP  T       5000.
OUTP  INTERM            MFIG              JOULES
METHOD                  NRRAO2
MOLECULAR WT.=  18.01528
DATA  V1     3656.65    V2     1594.78    V3     3755.79    X11    -45.18
DATA  X12    -15.14     X33    -44.62     X13    -165.48    X22    -17.04
DATA  Y233   -.81       Y333   -.45       X23    -19.99
DATA  Y111   .47        Y112   -.10       Y113   .68        Y122   -0.1
DATA  Y123   -1.72      Y133   1.17       Y222   -.60       Y223   1.55
DATA  A0     27.848     B0     14.5064    C0     9.28285    SYMNO 2.
DATA  ALFAA1 .750       ALFAA2 -2.941     ALFAA3 1.253      ALFAB1 .238
DATA  ALFAB2 -.160      ALFAB3 .078       ALFAC1 .2018      ALFAC2 .1392
DATA  ALFAC3 .1445      RHO    .0000213   STATWT 1.
FINISH
AI = 0.0325387    ALPHA A = 0.7500000    ALPHA B = 0.2380000    ALPHA C = 0.2018000    I =1
AI =-0.0508216    ALPHA A =-2.9410000    ALPHA B =-0.1600000    ALPHA C = 0.1392000    I =2
AI = 0.0329687    ALPHA A = 1.2529993    ALPHA B = 0.0779999    ALPHA C = 0.1445000    I =3
THETA(1) =    4.448227    THETA(2) =   19.370178    THETA(3) =    0.000000

A0= 27.847992     B0= 14.506399     C0=  9.282849

IAIBIC=       0.005849E-117 (G*CM**2)**3
Y(1,1,1) =  0.470    Y(1,1,2) = -0.100    Y(1,1,3) =  0.680    Y(1,2,2) = -0.100    Y(1,2,3) = -1.720
Y(1,3,3) =  1.170    Y(2,2,2) = -0.600    Y(2,2,3) =  1.550    Y(2,3,3) = -0.810    Y(3,3,3) = -0.450

X(I,J)
  -42.7750  -16.4000 -162.6400
  -16.4000  -19.0150  -19.3700
 -162.6400  -19.3700  -46.4650

V( 1) =3656.6499(1)      G =  0.000

V( 2) =1594.7798(1)      G =  0.000

V( 3) =3755.7898(1)      G =  0.000

T = 5000.000

   U = 0.1052215e+01   R = 0.3491637e+00   S = 0.1536484e+01   I = 1

   U = 0.4589038e+00   R = 0.6319761e+00   S = 0.2717215e+01   I = 2

   U = 0.1080742e+01   R = 0.3393437e+00   S = 0.1513646e+01   I = 3

CONTRIBUTION              Q              LN Q          H-H0/RT          CP/R
   ELEC           0.5000e+00      -0.69314718       0.00000000       0.00000000
   H.O.           0.6319e+01       1.84362507       1.90765095       2.80335808
   R.R.           0.5930e+04       8.68771458       1.50000000       1.50000000
   RHO            0.1112e+01       0.10649991       0.10649991       0.21299982
   THTA           0.1001e+01       0.00088938      -0.00089040       0.00000076

FIRST ORDER CORRECTIONS
   ALFA           0.9546e+00      -0.04642935      -0.04005833      -0.06193434
   XIJ            0.1071e+01       0.06857038       0.12646741       0.30334258
   YIJK           0.1004e+01       0.00428620       0.01142810       0.03873271
   AXIJ           0.9930e+00      -0.00702811      -0.01502087      -0.04562024

 SECOND ORDER CORRECTIONS
   XIJ2           0.1010e+01       0.00975084       0.02659326       0.09222138
   XY             0.1003e+01       0.00264854       0.00939406       0.04116780
   AX2            0.9977e+00      -0.00226233      -0.00755092      -0.03202931


ORIGINAL

ASSIGNED H AT   0 K = -238921.044 J/MOLE

      T          CP          H-H0          H-H298          S          -(G-H0)        -(G-H298)          H            -G
    DEG-K      J/MOL-K       J/MOL          J/MOL        J/MOL-K       J/MOL          J/MOL          J/MOL        J/MOL

  5000.00     61.13024    254611.490                    316.597784   1328377.430                   15690.446    1567298.474


              ORIGINAL          BAR
```

Example 6 (Mg(cr,ℓ) by Methods READIN and COEF with EFTAPE and LSQS Options)

Problem.—Process data for an assigned reference element to illustrate preparation of EF data. Select an element with more than one condensed phase in temperature range of interest. The solid phase is in the crystalline form and this is indicated on the NAME record as Mg(cr). Also obtain least-squares coefficients for each phase.

Magnesium in the solid and liquid phases was chosen to be the assigned reference element. Referring to the input data set, there is a NAME record for each phase. The information on these records will be included with the first record of the least-squares coefficients output on I/O units 6 and 10. See the section **NAME record** in appendix B and table VIII. The formula record contains the atomic symbol in the required capital letters, the integer 1 and the letter S in parentheses. The parentheses are a requirement for condensed species. As was noted in the section **Formula record**, the letter S must be used on the formula record of a reference element to specify the solid state. However, a more descriptive letter (or letters) such as cr may be used in the NAME record. Also included on the formula record is the assigned enthalpy at 298.15 K (HF298) which is 0 since this is a reference element. The CODA89 label on the DATE record was chosen to indicate a 1989 CODATA reference. The four REFN records give the full reference and some comments on the data.

The two OUTP records list many options. The EFTAPE label calls for the enthalpy and Gibbs energy data (EF data) to be merged in an unformatted form with the data on I/O unit 13 for use in calculating $\Delta_f H^o_T$ and $\log_{10} K$ values for future calculations. The data are also listed in formatted form on I/O units 11 and 6 (see the second to last table for this example printed in the output below). More discussion is given in the section **Saved Output** in appendix C. The LSQS label calls for least-squares coefficients. The MFIG label calls for many-figured tables with joules as the energy unit (JOULES). The CTAB label calls for a table to be listed for data calculated from the least-squares coefficients. The temperature schedule for the *coefficients* table is given on the CTEM record—namely, from 200 to 5000 K in 200 K intervals. Room temperature (298.15 K) and phase transition temperatures are always inserted by the PAC91 program in these schedules.

Data for the solid phase (Mg(s)) are processed by method READIN, whereas data for the liquid phase are processed by method COEF. The 18 data records (indicated by record ID MG- SOL) give data for the solid phase from 25 to 923 K. The melting point is given on the METHOD record as 923.. Also given on this record is the H298H0 value of 4998.. The unit of J/mol is specified by the label JOULES. Note that some of the enthalpy values are for H-H0 ($H^o_T - H^o_0$) whereas others are for H-H2 ($H^o_T - H^o_{298.15}$). This was done just to demonstrate some of the options available.

The heat of melting is given on the second METHOD record (method COEF for the liquid phase) as DELTAH = 8477. J/mol. The temperature schedule for thermodynamic functions calculated from read-in coefficients is given on the TEMP record preceding the COEF method record. Following this METHOD record are two data records for the liquid phase (records MG-LIQ). The first MG-LIQ record contains one coefficient (C1 = 34.309), one exponent (E1 = 0.), and the temperature range for which these coefficients are valid (923 to 6000 K). The PAC91 program automatically prepares and lists the read-in coefficients in the same format as the least-squares coefficients (see table VIII). The TCOEF label (on the second MG-LIQ data record for the liquid phase) has no temperature information following it. Therefore, the temperature range for the liquid phase on the coefficient output just discussed is taken to be the same as the input temperature range for the liquid.

As the listed output below shows, the least-squares calculations for the crystalline phase were done by PAC91 after reading the METHOD COEF record and before processing the liquid data records. This is evidenced by the intermediate output for the least-squares fit for the crystalline phase. Since no LSTSQS records were included in the input, the default parameters are used. The temperature interval starts at 200 K and ends at the 923 K transition which comes ahead of the 1000 K midpoint. The functions are fit simultaneously and constrained to fit at 298.15 K. The equation is the default seven-coefficient function for C^o_p (see eq. (17)). The record images described in table VIII are printed here (I/O unit 6) and on I/O unit 10.

This output is followed by the input data images for the liquid (record ID MG-LIQ). The TCOEF label indicates that the coefficients on the data records are to be included with the least-squares coefficients. In this case there is one coefficient for the constant C^o_p. The two required integration constants for enthalpy and entropy are calculated by PAC91 to fit the properties calculated from the least-squares coefficients for the solid phase at 923 K plus the heat of melting. These coefficients are also written on I/O unit 6 following the FINISH record as well as on I/O unit 10. No least-squares calculations were made for the liquid since the TCOEF option was used.

The final three tables are in order: the many-figured *original* table in SI units, the dimensionless EF data, and the many-figured *coefficient table* in SI units.

Input. - The input data set for Mg(cr,ℓ), example 6, is as follows:

	Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	Mg(cr)		Magnesium Hexagonal Crystal. CODATA 1989, p244. Expl.						6
a	NAME	Mg(l)		Magnesium Liquid. CODATA 1989, p244.						
	MGl(S)			HF298	0.					
	DATE	CODA89								
a	REFN	Cox,J.D.; Wagman,		D.D.; and Medvedev,V.A.:			CODATA Key Values for			
a	REFN	Thermodynamics.		Hemisphere Publ. Corp., 1989.						
a	REFN	CODATA S value at		75 K was obviously wrong and corrected by interpolation.						
a	REFN	H and S for crystal at 923 adjusted so rounded liq values match CODATA.								
	OUTP	EFTAPE		MFIG		JOULES		LSQS		
	OUTP	CTAB								
	CTEM	T	200.	I	200.	T	6000.			
	METHOD	READIN		H298H0	4998.	JOULES		MELTPT	923.	
	MG-SOL	T	25.	CP	0.781	S	.246	H-H0	5.	
	MG-SOL	T	50.	CP	5.740	S	2.104	H-H0	79.	
	MG-SOL	T	75.	CP	11.542	S	5.578	H-H0	297.	
	MG-SOL	T	100.	CP	15.762	S	9.505	H-H2	-4356.	
	MG-SOL	T	150.	CP	20.474	S	16.910	H-H0	1563.	
	MG-SOL	T	200.	CP	22.724	S	23.143	H-H2	-2349.	
	MG-SOL	T	250.	CP	24.018	S	28.364	H-H0	3820.	
	MG-SOL	T	298.15	CP	24.869	S	32.671	H-H2	0000.	
	MG-SOL	T	300.	CP	24.897	S	32.825	H-H2	46.	
	MG-SOL	T	350.	CP	25.568	S	36.715	H-H0	6306.	
	MG-SOL	T	400.	CP	26.144	S	40.167	H-H2	2601.	
	MG-SOL	T	450.	CP	26.668	S	43.277	H-H0	8920.	
	MG-SOL	T	500.	CP	27.171	S	46.113	H-H2	5268.	
	MG-SOL	T	600.	CP	28.184	S	51.156	H-H2	8035.	
	MG-SOL	T	700.	CP	29.279	S	55.581	H-H2	10907.	
	MG-SOL	T	800.	CP	30.507	S	59.569	H-H2	13895.	
	MG-SOL	T	900.	CP	31.895	S	63.241	H-H2	17014.	
	MG-SOL	T	923.	CP	32.238	S	64.0498	H-H2	17751.2	
	TEMP	T	923.	T	1000.	I	100.	T	6000.	
	METHOD	COEF		DELTAH	8477.	JOULES				
	MG-LIQ	T	923.	T	6000.	C1	34.309	E1	0.	
	MG-LIQ	TCOEF								
	FINISH									

[a]All alphanumeric characters.

Listed output. - Listed output for Mg(cr,ℓ), example 6, is as follows:

```
NAME  Mg(cr)            Magnesium Hexagonal Crystal. CODATA 1989, p244.  Expl. 6
NAME  Mg(l)             Magnesium Liquid.   CODATA 1989, p244.
MG1(S)                  HF298     0.
DATE  CODA89
REFN  Cox,J.D.; Wagman, D.D.; and Medvedev,V.A.: CODATA Key Values for
REFN    Thermodynamics.  Hemisphere Publ. Corp., 1989.
REFN  CODATA S value at 75 K was obviously wrong and corrected by interpolation.
REFN  H and S for crystal at 923 adjusted so rounded liq values match CODATA.
OUTP  EFTAPE            MFIG              JOULES            LSQS
OUTP  CTAB
CTEM  T      200.       I       200.      T       6000.
METHODREADIN            H298H0  4998.     JOULES            MELTPT  923.
MG-SOLT       25.       CP      0.781     S         .246    H-H0      5.
MG-SOLT       50.       CP      5.740     S        2.104    H-H0     79.
MG-SOLT       75.       CP     11.542     S        5.578    H-H0    297.
MG-SOLT      100.       CP     15.762     S        9.505    H-H2  -4356.
MG-SOLT      150.       CP     20.474     S       16.910    H-H0   1563.
MG-SOLT      200.       CP     22.724     S       23.143    H-H2  -2349.
MG-SOLT      250.       CP     24.018     S       28.364    H-H0   3820.
MG-SOLT      298.15     CP     24.869     S       32.671    H-H2   0000.
MG-SOLT      300.       CP     24.897     S       32.825    H-H2     46.
MG-SOLT      350.       CP     25.568     S       36.715    H-H0   6306.
MG-SOLT      400.       CP     26.144     S       40.167    H-H2   2601.
MG-SOLT      450.       CP     26.668     S       43.277    H-H0   8920.
MG-SOLT      500.       CP     27.171     S       46.113    H-H2   5268.
MG-SOLT      600.       CP     28.184     S       51.156    H-H2   8035.
MG-SOLT      700.       CP     29.279     S       55.581    H-H2  10907.
MG-SOLT      800.       CP     30.507     S       59.569    H-H2  13895.
MG-SOLT      900.       CP     31.895     S       63.241    H-H2  17014.
MG-SOLT      923.       CP     32.238     S       64.0498   H-H2  17751.2
TEMP  T       923.      T       1000.     I        100.     T      6000.
METHODCOEF              DELTAH  8477.     JOULES
```

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
200.00	2.7330534	2.7329970	1.5929983	1.5928976	2.7834473	2.7834025	1.1904490	1.1905050
	0.0000564	0.0000206	0.0001007	0.0000632	0.0000447	0.0000161	-0.0000560	-0.0000470
250.00	2.8886850	2.8889734	1.8377511	1.8377226	3.4113856	3.4113582	1.5736345	1.5736357
	-0.0002884	-0.0000998	0.0000286	0.0000155	0.0000274	0.0000080	-0.0000011	-0.0000007
298.15	2.9910362	2.9910362	2.0161590	2.0161590	3.9293957	3.9293957	1.9132367	1.9132367
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
300.00	2.9944038	2.9944025	2.0221677	2.0221811	3.9479176	3.9479080	1.9257499	1.9257263
	0.0000012	0.0000004	-0.0000135	-0.0000067	0.0000096	0.0000024	0.0000231	0.0000120
350.00	3.0751060	3.0755575	2.1669519	2.1670665	4.4157746	4.4158074	2.2488225	2.2487409
	-0.0004514	-0.0001468	-0.0001146	-0.0000529	-0.0000330	-0.0000075	0.0000816	0.0000363
400.00	3.1443825	3.1444155	2.2848610	2.2850201	4.8309522	4.8310806	2.5460911	2.5460605
	-0.0000330	-0.0000105	-0.0001590	-0.0000696	-0.0001285	-0.0000266	0.0000306	0.0000129
450.00	3.2074049	3.2072398	2.3840518	2.3840347	5.2049970	5.2051049	2.8209453	2.8210701
	0.0001651	0.0000515	0.0000170	0.0000071	-0.0001078	-0.0000207	-0.0001249	-0.0000443
500.00	3.2679015	3.2676623	2.4694179	2.4693854	5.5460875	5.5461580	3.0766696	3.0767727
	0.0002393	0.0000732	0.0000325	0.0000132	-0.0000705	-0.0000127	-0.0001031	-0.0000335
600.00	3.3897367	3.3896968	2.6125011	2.6125225	6.1526175	6.1526248	3.5401164	3.5401023
	0.0000399	0.0000118	-0.0000213	-0.0000082	-0.0000073	-0.0000012	0.0000141	0.0000040
700.00	3.5214342	3.5215153	2.7327442	2.7328045	6.6848197	6.6848772	3.9520755	3.9520727
	-0.0000811	-0.0000230	-0.0000604	-0.0000221	-0.0000576	-0.0000086	0.0000028	0.0000007
800.00	3.6691278	3.6690433	2.8403658	2.8404281	7.1644631	7.1645425	4.3240973	4.3241144
	0.0000845	0.0000230	-0.0000623	-0.0000219	-0.0000794	-0.0000111	-0.0000171	-0.0000040
900.00	3.8360649	3.8359739	2.9415778	2.9415776	7.6061007	7.6061272	4.6645229	4.6645496
	0.0000910	0.0000237	0.0000002	0.0000001	-0.0000265	-0.0000035	-0.0000267	-0.0000057
923.00	3.8773181	3.8773931	2.9643383	2.9643784	7.7033764	7.7034439	4.7390381	4.7390654
	-0.0000750	-0.0000193	-0.0000401	-0.0000135	-0.0000675	-0.0000088	-0.0000274	-0.0000053

```
MAX REL ERR CP/R  =  0.000147    TEMP =   350.     AVER REL ERR CP/R  =  0.000039     REL LST SQ ERR CP/R  =  0.000057
MAX REL ERR HH/RT =  0.000070    TEMP =   400.     AVER REL ERR HH/RT =  0.000023     REL LST SQ ERR HH/RT =  0.000032
MAX REL ERR S/R   =  0.000027    TEMP =   400.     AVER REL ERR S/R   =  0.000010     REL LST SQ ERR S/R   =  0.000012
MAX REL ERR GH/RT =  0.000047    TEMP =   200.     AVER REL ERR GH/RT =  0.000016     REL LST SQ ERR GH/RT =  0.000023
    MAX ERR CP/R  =  0.000451    TEMP.=   350.         AVER ERR CP/R  =  0.000124         LST SQ ERR CP/R  =  0.000177
    MAX ERR HH/RT =  0.000159    TEMP =   400.         AVER ERR HH/RT =  0.000050         LST SQ ERR HH/RT =  0.000068
    MAX ERR S/R   =  0.000128    TEMP =   400.         AVER ERR S/R   =  0.000051         LST SQ ERR S/R   =  0.000063
    MAX ERR GH/RT =  0.000125    TEMP =   450.         AVER ERR GH/RT =  0.000039         LST SQ ERR GH/RT =  0.000055
CP/R =   -7.3537794e+03T**-2.0  -6.9826242e+01T**-1.0   3.2083651e+00T** 0.0   2.2508743e-04T** 1.0   2.0515951e-07T** 2.0
         5.6911578e-10T** 3.0  -1.0573239e-13T** 4.0
(H-H0)/R CONSTANT =  0.48294728e+01, H/R CONSTANT =-0.59628833e+03, S/R CONSTANT =-0.14707183e+02
```

Mg(cr) Mg(l)

```
 THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

Mg(cr)            Magnesium Hexagonal Crystal. CODATA 1989, p244.  Expl. 6
 1 CODA89 MG  1.00     0.00     0.00     0.00     0.00 1      24.30500          0.000
    200.000   923.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          4998.000
 -7.35377939d+03 -6.98262416d+01  3.20836507d+00  2.25087426d-04  2.05159514d-07
  5.69115784d-10 -1.05732390d-13  0.00000000d+00 -5.96288332d+02 -1.47071833d+01

MG-LIQT      923.       T      6000.      C1      34.309     E1      0.

MG-LIQTCOEF

FINISH

COEFFICIENTS ADJUSTED TO FIT UPPER PHASE AT  923.00

 THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

Mg(l)             Magnesium Liquid.   CODATA 1989, p244.
 1 CODA89 MG  1.00     0.00     0.00     0.00     0.00 2      24.30500          0.000
    923.000  6000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0          4998.000
  4.12640071d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -6.54121412d+02 -1.93654933d+01



ORIGINAL          Mg(cr)            Mg(l)

ASSIGNED H AT   0 K =   -4998.000 J/MOLE

      T         CP          H-H0        H-H298          S          -(G-H0)     -(G-H298)         H           -G
    DEG-K     J/MOL-K      J/MOL        J/MOL       J/MOL-K       J/MOL        J/MOL         J/MOL       J/MOL

     25.00     0.78100         5.000    -4993.000     0.246000       1.150     4999.150    -4993.000    4999.150
     50.00     5.74000        79.000    -4919.000     2.104000      26.200     5024.200    -4919.000    5024.200
     75.00    11.54200       297.000    -4701.000     5 578000     121.350     5119.350    -4701.000    5119.350
    100.00    15.76200       642.000    -4356.000     9.505000     308.500     5306.500    -4356.000    5306.500
    150.00    20.47400      1563.000    -3435.000    16.910000     973.500     5971.500    -3435.000    5971.500
    200.00    22.72400      2649.000    -2349.000    23.143000    1979.600     6977.600    -2349.000    6977.600
    250.00    24.01800      3820.000    -1178.000    28.364000    3271.000     8269.000    -1178.000    8269.000
    298.15    24.86900      4998.000        0.000    32.671000    4742.859     9740.859        0.000    9740.859
    300.00    24.89700      5044.000       46.000    32.825000    4803.500     9801.500       46.000    9801.500
    350.00    25.56800      6306.000     1308.000    36.715000    6544.250    11542.250     1308.000   11542.250
    400.00    26.14400      7599.000     2601.000    40.167000    8467.800    13465.800     2601.000   13465.800
    450.00    26.66800      8920.000     3922.000    43.277000   10554.650    15552.650     3922.000   15552.650
    500.00    27.17100     10266.000     5268.000    46.113000   12790.500    17788.500     5268.000   17788.500
    600.00    28.18400     13033.000     8035.000    51.156000   17660.600    22658.600     8035.000   22658.600
    700.00    29.27900     15905.000    10907.000    55.581000   23001.700    27999.700    10907.000   27999.700
    800.00    30.50700     18893.000    13895.000    59.569000   28762.200    33760.200    13895.000   33760.200
    900.00    31.89500     22012.000    17014.000    63.241000   34904.900    39902.900    17014.000   39902.900
    923.00    32.23800     22749.200    17751.200    64.049800   36368.765    41366.765    17751.200   41366.765
    923.00    34.30900     31226.200    26228.200    73.233982   36368.765    41366.765    26228.200   41366.765
   1000.00    34.30900     33867.993    28869.993    75.983026   42115.033    47113.033    28869.993   47113.033
   1100.00    34.30900     37298.893    32300.893    79.253023   49879.433    54877.433    32300.893   54877.433
   1200.00    34.30900     40729.793    35731.793    82.238297   57956.163    62954.163    35731.793   62954.163
   1300.00    34.30900     44160.693    39162.693    84.984482   66319.134    71317.134    39162.693   71317.134
   1400.00    34.30900     47591.593    42593.593    87.527052   74946.280    79944.280    42593.593   79944.280
   1500.00    34.30900     51022.493    46024.493    89.894129   83818.700    88816.700    46024.493   88816.700
   1600.00    34.30900     54453.393    49455.393    92.108381   92920.017    97918.017    49455.393   97918.017
   1700.00    34.30900     57884.293    52886.293    94.188351  102235.904   107233.904    52886.293  107233.904
   1800.00    34.30900     61315.193    56317.193    96.149399  111753.725   116751.725    56317.193  116751.725
   1900.00    34.30900     64746.093    59748.093    98.004391  121462.251   126460.251    59748.093  126460.251
   2000.00    34.30900     68176.993    63178.993    99.764213  131351.433   136349.433    63178.993  136349.433
   2100.00    34.30900     71607.893    66609.893   101.438155  141412.232   146410.232    66609.893  146410.232
   2200.00    34.30900     75038.793    70040.793   103.034210  151636.469   156634.469    70040.793  156634.469
   2300.00    34.30900     78469.693    73471.693   104.559306  162016.710   167014.710    73471.693  167014.710
   2400.00    34.30900     81900.593    76902.593   106.019483  172546.167   177544.167    76902.593  177544.167
   2500.00    34.30900     85331.493    80333.493   107.420045  183218.620   188216.620    80333.493  188216.620
   2600.00    34.30900     88762.393    83764.393   108.765669  194028.345   199026.345    83764.393  199026.345
   2700.00    34.30900     92193.293    87195.293   110.060502  204970.061   209968.061    87195.293  209968.061
   2800.00    34.30900     95624.193    90626.193   111.308239  216038.876   221036.876    90626.193  221036.876
   2900.00    34.30900     99055.093    94057.093   112.512187  227230.250   232228.250    94057.093  232228.250
   3000.00    34.30900    102485.993    97487.993   113.675315  238539.953   243537.953    97487.993  243537.953
   3100.00    34.30900    105916.893   100918.893   114.800302  249964.042   254962.042   100918.893  254962.042
   3200.00    34.30900    109347.793   104349.793   115.889568  261498.823   266496.823   104349.793  266496.823
   3300.00    34.30900    112778.693   107780.693   116.945312  273140.838   278138.838   107780.693  278138.838
   3400.00    34.30900    116209.593   111211.593   117.969538  284886.835   289884.835   111211.593  289884.835
   3500.00    34.30900    119640.493   114642.493   118.964071  296733.756   301731.756   114642.493  301731.756
   3600.00    34.30900    123071.393   118073.393   119.930586  308678.716   313676.716   118073.393  313676.716
   3700.00    34.30900    126502.293   121504.293   120.870617  320718.991   325716.991   121504.293  325716.991
   3800.00    34.30900    129933.193   124935.193   121.785578  332852.004   337850.004   124935.193  337850.004
   3900.00    34.30900    133364.093   128366.093   122.676771  345075.314   350073.314   128366.093  350073.314
   4000.00    34.30900    136794.993   131796.993   123.545400  357386.606   362384.606   131796.993  362384.606
   4100.00    34.30900    140225.893   135227.893   124.392579  369783.679   374781.679   135227.893  374781.679
   4200.00    34.30900    143656.793   138658.793   125.219341  382264.441   387262.441   138658.793  387262.441
   4300.00    34.30900    147087.693   142089.693   126.026649  394826.899   399824.899   142089.693  399824.899
   4400.00    34.30900    150518.593   145520.593   126.815397  407469.152   412467.152   145520.593  412467.152
   4500.00    34.30900    153949.493   148951.493   127.586418  420189.387   425187.387   148951.493  425187.387
   4600.00    34.30900    157380.393   152382.393   128.340492  432985.871   437983.871   152382.393  437983.871
   4700.00    34.30900    160811.293   155813.293   129.078349  445856.945   450854.945   155813.293  450854.945
   4800.00    34.30900    164242.193   159244.193   129.800670  458801.023   463799.023   159244.193  463799.023
   4900.00    34.30900    167673.093   162675.093   130.508097  471816.583   476814.583   162675.093  476814.583
   5000.00    34.30900    171103.993   166105.993   131.201232  484902.166   489900.166   166105.993  489900.166
   5100.00    34.30900    174534.893   169536.893   131.880640  498056.372   503054.372   169536.893  503054.372
   5200.00    34.30900    177965.793   172967.793   132.546855  511277.854   516275.854   172967.793  516275.854
   5300.00    34.30900    181396.693   176398.693   133.200380  524565.320   529563.320   176398.693  529563.320
   5400.00    34.30900    184827.593   179829.593   133.841688  537917.523   542915.523   179829.593  542915.523
   5500.00    34.30900    188258.493   183260.493   134.471229  551333.265   556331.265   183260.493  556331.265
   5600.00    34.30900    191689.393   186691.393   135.089426  564811.391   569809.391   186691.393  569809.391
   5700.00    34.30900    195120.293   190122.293   135.696680  578350.786   583348.786   190122.293  583348.786
   5800.00    34.30900    198551.193   193553.193   136.293374  591950.375   596948.375   193553.193  596948.375
   5900.00    34.30900    201982.093   196984.093   136.879867  605609.120   610607.120   196984.093  610607.120
   6000.00    34.30900    205412.993   200414.993   137.456502  619326.020   624324.020   200414.993  624324.020



                ORIGINAL          Mg(cr)            Mg(l)
```

EFDA MG1S CODA89 H0/R -601.1178MP 923.0000NT 70.0000

25.00	0.024054	0.005532	50.00	0.190029	0.063022
75.00	0.476276	0.194600	100.00	0.772144	0.371038
150.00	1.253231	0.780563	200.00	1.592998	1.190449
250.00	1.837751	1.573635	298.15	2.016159	1.913237
360.00	2.022168	1.925750	350.00	2.166952	2.248822
400.00	2.284861	2.546091	450.00	2.384052	2.820945
500.00	2.469418	3.076670	600.00	2.612501	3.540116
700.00	2.732744	3.952076	800.00	2.840366	4.324097
900.00	2.941578	4.664523	923.00	2.964338	4.739038
923.00	4.068935	4.739038	1000.00	4.073360	5.065245
1100.00	4.078182	5.453712	1200.00	4.082200	5.808737
1300.00	4.085600	6.135625	1400.00	4.088515	6.438510
1500.00	4.091040	6.720677	1600.00	4.093250	6.984778
1700.00	4.095200	7.232990	1800.00	4.096934	7.467115
1900.00	4.098485	7.688667	2000.00	4.099880	7.898928
2100.00	4.101143	8.098993	2200.00	4.102291	8.289805
2300.00	4.103340	8.472183	2400.00	4.104300	8.646840
2500.00	4.105184	8.814404	2600.00	4.106000	8.975428
2700.00	4.106756	9.130404	2800.00	4.107458	9.279770
2900.00	4.108111	9.423918	3000.00	4.108720	9.563199
3100.00	4.109291	9.697933	3200.00	4.109826	9.828406
3300.00	4.110328	9.954880	3400.00	4.110801	10.077593
3500.00	4.111246	10.196761	3600.00	4.111667	10.312585
3700.00	4.112065	10.425246	3800.00	4.112443	10.534912
3900.00	4.112801	10.641740	4000.00	4.113141	10.745871
4100.00	4.113464	10.847439	4200.00	4.113772	10.946567
4300.00	4.114066	11.043370	4400.00	4.114346	11.137953
4500.00	4.114614	11.230418	4600.00	4.114870	11.320855
4700.00	4.115115	11.409353	4800.00	4.115351	11.495993
4900.00	4.115576	11.580851	5000.00	4.115793	11.663999
5100.00	4.116001	11.745504	5200.00	4.116201	11.825431
5300.00	4.116393	11.903839	5400.00	4.116578	11.980785
5500.00	4.116757	12.056322	5600.00	4.116929	12.130502
5700.00	4.117095	12.203371	5800.00	4.117256	12.274976
5900.00	4.117411	12.345359	6000.00	4.117561	12.414562

ORIGINAL Mg(cr) Mg(l)

COEFFICIENTS Mg(cr) Mg(l)

ASSIGNED H AT 0 K = -4998.000 J/MOLE

T DEG-K	CP J/MOL-K	H-H0 J/MOL	H-H298 J/MOL	S J/MOL-K	-(G-H0) J/MOL	-(G-H298) J/MOL	H J/MOL	-G J/MOL
200.00	22.72353	2648.833	-2349.167	23.142628	1979.693	6977.693	-2349.167	6977.693
298.15	24.86900	4998.000	0.000	32.671000	4742.859	9740.859	0.000	9740.859
400.00	26.14427	7599.529	2601.529	40.168068	8467.698	13465.698	2601.529	13465.698
600.00	28.18367	13033.106	8035.106	51.156060	17660.530	22658.530	8035.106	22658.530
800.00	30.50630	18893.414	13895.414	59.569660	28762.314	33760.314	13895.414	33760.314
923.00	32.23862	22749.508	17751.508	64.050361	36368.975	41366.975	17751.508	41366.975
923.00	34.30900	31226.508	26228.508	73.234543	36368.975	41366.975	26228.508	41366.975
1000.00	34.30900	33868.301	28870.301	75.983588	42115.287	47113.287	28870.301	47113.287
1200.00	34.30900	40730.101	35732.101	82.238858	57956.529	62954.529	35732.101	62954.529
1400.00	34.30900	47591.901	42593.901	87.527614	74946.758	79944.758	42593.901	79944.758
1600.00	34.30900	54453.701	49455.701	92.108942	92920.607	97918.607	49455.701	97918.607
1800.00	34.30900	61315.501	56317.501	96.149960	111754.428	116752.428	56317.501	116752.428
2000.00	34.30900	68177.301	63179.301	99.764774	131352.248	136350.248	63179.301	136350.248
2200.00	34.30900	75039.101	70041.101	103.034771	151637.396	156635.396	70041.101	156635.396
2400.00	34.30900	81900.901	76902.901	106.020045	172547.206	177545.206	76902.901	177545.206
2600.00	34.30900	88762.701	83764.701	108.766230	194029.497	199027.497	83764.701	199027.497
2800.00	34.30900	95624.501	90626.501	111.308800	216040.140	221038.140	90626.501	221038.140
3000.00	34.30900	102486.301	97488.301	113.675877	238541.329	243539.329	97488.301	243539.329
3200.00	34.30900	109348.101	104350.101	115.890129	261500.312	266498.312	104350.101	266498.312
3400.00	34.30900	116209.901	111211.901	117.970099	284888.436	289886.436	111211.901	289886.436
3600.00	34.30900	123071.701	118073.701	119.931147	308680.428	313678.428	118073.701	313678.428
3800.00	34.30900	129933.501	124935.501	121.786139	332853.829	337851.829	124935.501	337851.829
4000.00	34.30900	136795.301	131797.301	123.545961	357388.543	362386.543	131797.301	362386.543
4200.00	34.30900	143657.101	138659.101	125.219903	382266.491	387264.491	138659.101	387264.491
4400.00	34.30900	150518.901	145520.901	126.815958	407471.314	412469.314	145520.901	412469.314
4600.00	34.30900	157380.701	152382.701	128.341053	432988.145	437986.145	152382.701	437986.145
4800.00	34.30900	164242.501	159244.501	129.801231	458803.409	463801.409	159244.501	463801.409
5000.00	34.30900	171104.301	166106.301	131.201793	484904.665	489902.665	166106.301	489902.665
5200.00	34.30900	177966.101	172968.101	132.547417	511280.465	516278.465	172968.101	516278.465
5400.00	34.30900	184827.901	179829.901	133.842249	537920.246	542918.246	179829.901	542918.246
5600.00	34.30900	191689.701	186691.701	135.089987	564814.226	569812.226	186691.701	569812.226
5800.00	34.30900	198551.501	193553.501	136.293935	591953.322	596951.322	193553.501	596951.322
6000.00	34.30900	205413.301	200415.301	137.457063	619329.079	624327.079	200415.301	624327.079

COEFFICIENTS Mg(cr) Mg(l)

Example 7 (MgO(g) by Method JANAF with LSQS and LOGK Options)

Problem.—Calculate thermodynamic functions for a species with excited electronic states using method JANAF. Obtain least-squares coefficients and tables with $\Delta_f H_T^o$ and $\log_{10} K$ columns.

Except for the missing TEMP records, the LOGK label on the OUTP record, and the data records, the input is similar to that in the previous examples. With no TEMP records, PAC91 uses the default temperature schedule of 100 (100) 6000 K and $T = 298.15$ K. LOGK calls for rounded tables with columns for $\Delta_f H_T^o$ and $\log_{10} K$. The data records are for 15 electronic states including the ground state as indicated by the numbers in columns 79 and 80. The excitation energies are given by the T0 numerical values. The remaining labels are defined in table VII. Since no statistical weight was given for the ground state PAC91 assigns a value of 1.

As with the last example, with LSQS on the OUTP record and no LSTSQS records, all the default temperature ranges, constraints, and exponents in equation (11) are set by the program. The default temperature range is 200 to 1000 K for the first interval and 1000 to 6000 K for the second interval. The default constraint temperature is 298.15 K for the first interval and 1000 K for the second interval. This may be seen in the least-squares output table where the errors at 298.15 K are zero and the values of the thermodynamic functions are identical at 1000 K for both the first and second intervals.

Finally, the last two tables in the output are rounded and include columns for $\Delta_f H_T^o$ and $\log_{10} K$. One table contains the original data and the other contains data calculated from the least-squares coefficients. Both used the EF data for Mg stored in example 6.

Input. - The input data set for MgO, example 7, is as follows:

[a]

Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
NAME	MGO		Magnesium Oxide.		JANAF	Dec.1974, pl	472.	Expl.	7
MG101			HF298	58158.	JOULES				
DATE	J12/74								
OUTP	JOULES		LOGK		CTAB		LSQS		
CTEM	T	200.	I	100.	T	1000.	I	200.	
CTEM	T	3000.							
METH	JANAF								
DATA	WE	785.1	WEXE	5.18	BE	.5743	ALPHA1	.0050	1
DATA	STATWT	6.	T0	2300.	WE	664.4	WEXE	3.9	2
DATA	BE	.5050	ALPHA1	.004					2
DATA	STATWT	2.	T0	3503.3	WE	664.4	WEXE	3.9	3
DATA	BE	.5050	ALPHA1	.004					3
DATA	STATWT	3.	T0	14000.	WE	824.1	WEXE	4.8	4
DATA	BE	.5822	ALPHA1	.0045					4
DATA	STATWT	1.	T0	20004.	WE	824.1	WEXE	4.76	5
DATA	BE	.5822	ALPHA1	.0045					5
DATA	STATWT	3.	T0	28000.	WE	632.5	WEXE	5.3	6
DATA	BE	.501	ALPHA1	.0048					6
DATA	STATWT	6.	T0	29000.	WE	632.5	WEXE	5.3	7
DATA	BE	.501	ALPHA1	.0048					7
DATA	STATWT	2.	T0	29775.	WE	632.5	WEXE	5.3	8
DATA	BE	.5014	ALPHA1	.0048					8
DATA	STATWT	3.	T0	30000.	WE	632.5	WEXE	5.3	9
DATA	BE	.501	ALPHA1	.0048					9
DATA	STATWT	1.	T0	30004.	WE	632.4	WEXE	5.2	10
DATA	BE	.5008	ALPHA1	.0048					10
DATA	STATWT	1.	T0	37684.	WE	632.4	WEXE	5.2	11
DATA	BE	.5273	ALPHA1	.0048					11
DATA	STATWT	6.	T0	37000.	WE	710.	WEXE	5.	12
DATA	BE	.5615	ALPHA1	.005					12
DATA	STATWT	2.	T0	37879.	WE	710.	WEXE	5.	13
DATA	BE	.5615	ALPHA1	.005					13
DATA	STATWT	6.	T0	39000.	WE	790.	WEXE	5.	14
DATA	BE	.5249	ALPHA1	.005					14
DATA	STATWT	2.	T0	39868.	WE	790.	WEXE	5.	15
DATA	BE	.5249	ALPHA1	.005					15
FINISH									

[a]All alphanumeric characters.

Listed output. - Listed output for MgO, example 7, is as follows:

```
NAME  MGO              Magnesium Oxide.  JANAF Dec.1974, p1472.          Expl. 7
MG101                  HF298     58158.  JOULES
DATE  J12/74
OUTP  JOULES           LOGK              CTAB              LSQS
CTEM  T        200.    I       100.      T     1000.       I       200.
CTEM  T       3000.
METH  JANAF
MOLECULAR WT.=  40.30440
DATA  WE       785.1   WEXE     5.18     BE       .5743   ALPHA1   .0050     1
DATA  STATWT    6.     TO      2300.     WE      664.4    WEXE     3.9       2
DATA  BE        .5050  ALPHA1      .004                                      2
DATA  STATWT    2.     TO      3503.3    WE      664.4    WEXE     3.9       3
DATA  BE        .5050  ALPHA1      .004                                      3
DATA  STATWT    3.     TO      14000.    WE      824.1    WEXE     4.8       4
DATA  BE        .5822  ALPHA1      .0045                                     4
DATA  STATWT    1.     TO      20004.    WE      824.1    WEXE     4.76      5
DATA  BE        .5822  ALPHA1      .0045                                     5
DATA  STATWT    3.     TO      28000.    WE      632.5    WEXE     5.3       6
DATA  BE        .501   ALPHA1      .0048                                     6
DATA  STATWT    6.     TO      29000.    WE      632.5    WEXE     5.3       7
DATA  BE        .501   ALPHA1      .0048                                     7
DATA  STATWT    2.     TO      29775.    WE      632.5    WEXE     5.3       8
DATA  BE        .5014  ALPHA1      .0048                                     8
DATA  STATWT    3.     TO      30000.    WE      632.5    WEXE     5.3       9
DATA  BE        .501   ALPHA1      .0048                                     9
                                 BAR    MGO


DATA  STATWT    1.     TO      30004.    WE      632.4    WEXE     5.2       10
DATA  BE        .5008  ALPHA1      .0048                                     10
DATA  STATWT    1.     TO      37684.    WE      632.4    WEXE     5.2       11
DATA  BE        .5273  ALPHA1      .0048                                     11
DATA  STATWT    6.     TO      37000.    WE      710.     WEXE     5.        12
DATA  BE        .5615  ALPHA1      .005                                      12
DATA  STATWT    2.     TO      37879.    WE      710.     WEXE     5.        13
DATA  BE        .5615  ALPHA1      .005                                      13
DATA  STATWT    6.     TO      39000.    WE      790.     WEXE     5.        14
DATA  BE        .5249  ALPHA1      .005                                      14
DATA  STATWT    2.     TO      39868.    WE      790.     WEXE     5.        15
DATA  BE        .5249  ALPHA1      .005                                      15
FINISH


                                 BAR    MGO
```

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
200.00	3.6222350	3.6230253	3.5211248	3.5245108	24.1596692	24.1625724	20.6385444	20.6380617
	-0.0007903	-0.0002182	-0.0033859	-0.0009616	-0.0029032	-0.0001202	0.0004827	0.0000234
298.15	3.8695880	3.8695880	3.5939207	3.5939207	25.6505882	25.6505882	22.0566675	22.0566675
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
300.00	3.8745991	3.8746711	3.5956373	3.5956363	25.6745422	25.6745402	22.0789049	22.0789039
	-0.0000719	-0.0000186	0.0000010	0.0000003	0.0000020	0.0000001	0.0000010	0.0000009
400.00	4.1834225	4.1808965	3.7020302	3.7017295	26.8292628	26.8289409	23.1272326	23.1272114
	0.0025260	0.0006038	0.0003007	0.0000812	0.0003219	0.0000120	0.0000212	0.0000069
500.00	4.6225831	4.6241862	3.8397236	3.8393366	27.8071580	27.8066531	23.9674344	23.9673165
	-0.0016032	-0.0003468	0.0003369	0.0001008	0.0005049	0.0000182	0.0001179	0.0000049
600.00	5.1811418	5.1827699	4.0157194	4.0157747	28.6981979	28.6981068	24.6824784	24.6823321
	-0.0016281	-0.0003142	-0.0000553	-0.0000138	0.0000911	0.0000032	0.0001463	0.0000059
700.00	5.7472747	5.7457533	4.2233515	4.2233775	29.5401461	29.5400372	25.3167947	25.3166597
	0.0015214	0.0002647	-0.0000260	-0.0000062	0.0001089	0.0000037	0.0001349	0.0000053
800.00	6.2013558	6.2012364	4.4438496	4.4437241	30.3389662	30.3386969	25.8951166	25.8949723
	0.0001194	0.0000192	0.0001255	0.0000282	0.0002693	0.0000089	0.0001438	0.0000056
900.00	6.4815119	6.4823453	4.6563835	4.6563580	31.0873489	31.0871685	26.4309654	26.4308104
	-0.0008335	-0.0001286	0.0000255	0.0000055	0.0001804	0.0000058	0.0001550	0.0000059
1000.00	6.5903910	6.5901425	4.8456316	4.8455819	31.7772400	31.7770331	26.9316084	26.9314511
	0.0002485	0.0000377	0.0000497	0.0000103	0.0002070	0.0000065	0.0001573	0.0000058

MAX REL ERR CP/R = 0.000604 TEMP = 400.
MAX REL ERR HH/RT = 0.000962 TEMP = 200.
MAX REL ERR S/R = 0.000120 TEMP = 200.
MAX REL ERR GH/RT = 0.000023 TEMP = 200.
MAX ERR CP/R = 0.002526 TEMP = 400.
MAX ERR HH/RT = 0.003386 TEMP = 200.
MAX ERR S/R = 0.002903 TEMP = 200.
MAX ERR GH/RT = 0.000483 TEMP = 200.

AVER REL ERR CP/R = 0.000195
AVER REL ERR HH/RT = 0.000121
AVER REL ERR S/R = 0.000018
AVER REL ERR GH/RT = 0.000006
AVER ERR CP/R = 0.000934
AVER ERR HH/RT = 0.000436
AVER ERR S/R = 0.000459
AVER ERR GH/RT = 0.000136

REL LST SQ ERR CP/R = 0.000268
REL LST SQ ERR HH/RT = 0.000307
REL LST SQ ERR S/R = 0.000039
REL LST SQ ERR GH/RT = 0.000009
LST SQ ERR CP/R = 0.001238
LST SQ ERR HH/RT = 0.001083
LST SQ ERR S/R = 0.000946
LST SQ ERR GH/RT = 0.000189

CP/R = 3.7782309e+05T**-2.0 -6.0817323e+03T**-1.0 4.1615823e+01T** 0.0 -1.1851989e-01T** 1.0 1.9434161e-04T** 2.0
-1.4549526e-07T** 3.0 4.0351763e-11T** 4.0

(H-H0)/R CONSTANT = 0.28401570e+05, H/R CONSTANT = 0.34324803e+05, S/R CONSTANT =-0.20182814e+03

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
1000.00	6.5903910	6.5901425	4.8456316	4.8455819	31.7772400	31.7770331	26.9316084	26.9314511
	0.0002485	0.0000377	0.0000497	0.0000103	0.0002070	0.0000065	0.0001573	0.0000058
1100.00	6.5678619	6.5718199	5.0040302	5.0043389	32.4051630	32.4053238	27.4011327	27.4009849
	-0.0039580	-0.0006026	-0.0003086	-0.0000617	-0.0001608	-0.0000050	0.0001478	0.0000054
1200.00	6.4621804	6.4608150	5.1303682	5.1307549	32.9725516	32.9728243	27.8421834	27.8420694
	0.0013655	0.0002113	-0.0003867	-0.0000754	-0.0002727	-0.0000083	0.0001140	0.0000041
1300.00	6.3137782	6.3101469	5.2272787	5.2274152	33.4841208	33.4841648	28.2568421	28.2567496
	0.0036313	0.0005751	-0.0001365	-0.0000261	-0.0000441	-0.0000013	0.0000925	0.0000033
1400.00	6.1506734	6.1480945	5.2990894	5.2989786	33.9460831	33.9458801	28.6469937	28.6469015
	0.0025789	0.0004193	0.0001108	0.0000209	0.0002030	0.0000060	0.0000922	0.0000032
1500.00	5.9898031	5.9895149	5.3504543	5.3502549	34.3649022	34.3646003	29.0144479	29.0143453
	0.0002882	0.0000481	0.0001994	0.0000373	0.0003019	0.0000088	0.0001025	0.0000035
1600.00	5.8401423	5.8418349	5.3856640	5.3855255	34.7466245	34.7463701	29.3609605	29.3608446
	-0.0016926	-0.0002898	0.0001385	0.0000257	0.0002544	0.0000073	0.0001160	0.0000039
1700.00	5.7056142	5.7083273	5.4083633	5.4083672	35.0965646	35.0964475	29.6882013	29.6880803
	-0.0027131	-0.0004755	-0.0000039	-0.0000007	0.0001171	0.0000033	0.0001210	0.0000041
1800.00	5.5871912	5.5899504	5.4215136	5.4216733	35.4192597	35.4193034	29.9977462	29.9976301
	-0.0027591	-0.0004938	-0.0001598	-0.0000295	-0.0000437	-0.0000012	0.0001161	0.0000039
1900.00	5.4843087	5.4863980	5.4274607	5.4277417	35.7185218	35.7186974	30.2910611	30.2909557
	-0.0020893	-0.0003810	-0.0002810	-0.0000518	-0.0001756	-0.0000049	0.0001054	0.0000035
2000.00	5.3956638	5.3967080	5.4280310	5.4283770	35.9975185	35.9977755	30.5694876	30.5693985
	-0.0010442	-0.0001935	-0.0003460	-0.0000637	-0.0002570	-0.0000071	0.0000890	0.0000029
2100.00	5.3196868	5.3196147	5.4246340	5.4249861	36.2588887	36.2591679	30.8342547	30.8341818
	0.0000721	0.0000135	-0.0003521	-0.0000649	-0.0002792	-0.0000077	0.0000729	0.0000024
2200.00	5.2548048	5.2537533	5.4183512	5.4186597	36.5048226	36.5050755	31.0864715	31.0864159
	0.0010516	0.0002001	-0.0003085	-0.0000569	-0.0002529	-0.0000069	0.0000556	0.0000013
2300.00	5.1995323	5.1977745	5.4100046	5.4102395	36.7371545	36.7373450	31.3271499	31.3271055
	0.0017577	0.0003381	-0.0002348	-0.0000434	-0.0001905	-0.0000052	0.0000444	0.0000014
2400.00	5.1525519	5.1504084	5.4002295	5.4003721	36.9574251	36.9575310	31.5571957	31.5571589
	0.0021435	0.0004160	-0.0001427	-0.0000264	-0.0001059	-0.0000029	0.0000368	0.0000012
2500.00	5.1127103	5.1104947	5.3895044	5.3895523	37.1669325	37.1669483	31.7774281	31.7773961
	0.0022156	0.0004333	-0.0000479	-0.0000089	-0.0000158	-0.0000004	0.0000320	0.0000010
2600.00	5.0790145	5.0769959	5.3781910	5.3781561	37.3667814	37.3667136	31.9885904	31.9885575
	0.0020186	0.0003974	0.0000349	0.0000065	0.0000678	0.0000018	0.0000329	0.0000010
2700.00	5.0506094	5.0489979	5.3665705	5.3664678	37.5579187	37.5577801	32.1913482	32.1913122
	0.0016115	0.0003191	0.0001027	0.0000191	0.0001386	0.0000037	0.0000360	0.0000011
2800.00	5.0267711	5.0257060	5.3548470	5.3547008	37.7411535	37.7409661	32.3863065	32.3862653
	0.0010651	0.0002119	0.0001462	0.0000273	0.0001874	0.0000050	0.0000412	0.0000013
2900.00	5.0068916	5.0064360	5.3431807	5.3430132	37.9171920	37.9169778	32.5740114	32.5739646
	0.0004556	0.0000910	0.0001675	0.0000313	0.0002143	0.0000057	0.0000468	0.0000014
3000.00	4.9904468	4.9906046	5.3316879	5.3315213	38.0866465	38.0864279	32.7549586	32.7549066
	-0.0001577	-0.0000316	0.0001667	0.0000313	0.0002186	0.0000057	0.0000519	0.0000016
3100.00	4.9770043	4.9777187	5.3204565	5.3203088	38.2500543	38.2498514	32.9295978	32.9295426
	-0.0007144	-0.0001435	0.0001477	0.0000278	0.0002030	0.0000053	0.0000553	0.0000017
3200.00	4.9661894	4.9673659	5.3095484	5.3094350	38.4078906	38.4077178	33.0983422	33.0982823
	-0.0011766	-0.0002369	0.0001134	0.0000214	0.0001728	0.0000045	0.0000594	0.0000018
3300.00	4.9576880	4.9592038	5.2990103	5.2989404	38.5605739	38.5604417	33.2615636	33.2615013
	-0.0015158	-0.0003057	0.0000698	0.0000132	0.0001322	0.0000034	0.0000624	0.0000019
3400.00	4.9512419	4.9529514	5.2888708	5.2888519	38.7084752	38.7083913	33.4196044	33.4195395
	-0.0017095	-0.0003453	0.0000190	0.0000036	0.0000839	0.0000022	0.0000649	0.0000019
3500.00	4.9466200	4.9483804	5.2791548	5.2791856	38.8519289	38.8518954	33.5727741	33.5727093
	-0.0017604	-0.0003559	-0.0000308	-0.0000058	0.0000335	0.0000009	0.0000643	0.0000019
3600.00	4.9436377	4.9453076	5.2698727	5.2699506	38.9912333	38.9912492	33.7213606	33.7212986
	-0.0016699	-0.0003378	-0.0000780	-0.0000148	-0.0000159	-0.0000004	0.0000620	0.0000018
3700.00	4.9421373	4.9435882	5.2610321	5.2611504	39.1266625	39.1267192	33.8656304	33.8655683
	-0.0014508	-0.0002936	-0.0001182	-0.0000225	-0.0000567	-0.0000014	0.0000615	0.0000018
3800.00	4.9419801	4.9431088	5.2526350	5.2527845	39.2584538	39.2585470	34.0058188	34.0057625
	-0.0011287	-0.0002284	-0.0001495	-0.0000285	-0.0000932	-0.0000024	0.0000563	0.0000017
3900.00	4.9430465	4.9437827	5.2446814	5.2448504	39.3868366	39.3869530	34.1421553	34.1421023
	-0.0007362	-0.0001489	-0.0001690	-0.0000322	-0.0001163	-0.0000030	0.0000527	0.0000015
4000.00	4.9452504	4.9455440	5.2371664	5.2373435	39.5120094	39.5121387	34.2748430	34.2747952
	-0.0002937	-0.0000594	-0.0001771	-0.0000338	-0.0001293	-0.0000033	0.0000478	0.0000014

BAR MGO

4100.00	4.9485103	4.9483438	5.2300825	5.2302585	39.6341581	39.6342894	34.4040756	34.4040309
	0.0001665	0.0000336	-0.0001760	-0.0000337	-0.0001313	-0.0000033	0.0000447	0.0000013
4200.00	4.9527482	4.9521454	5.2234278	5.2235896	39.7534544	39.7535760	34.5300266	34.5299865
	0.0006028	0.0001217	-0.0001618	-0.0000310	-0.0001216	-0.0000031	0.0000402	0.0000012
4300.00	4.9579160	4.9569212	5.2171907	5.2173306	39.8700514	39.8701565	34.6528606	34.6528260
	0.0009947	0.0002006	-0.0001398	-0.0000268	-0.0001052	-0.0000026	0.0000347	0.0000010
4400.00	4.9639549	4.9626494	5.2113657	5.2114755	39.9841010	39.9841776	34.7727353	34.7727021
	0.0013055	0.0002630	-0.0001098	-0.0000211	-0.0000766	-0.0000019	0.0000332	0.0000010
4500.00	4.9708240	4.9693107	5.2059412	5.2060183	40.0957288	40.0957753	34.8897876	34.8897570
	0.0015133	0.0003044	-0.0000771	-0.0000148	-0.0000465	-0.0000012	0.0000306	0.0000009
4600.00	4.9784954	4.9768861	5.2009125	5.2009532	40.2050650	40.2050766	35.0041526	35.0041234
	0.0016093	0.0003232	-0.0000407	-0.0000078	-0.0000116	-0.0000003	0.0000292	0.0000008
4700.00	4.9869234	4.9853543	5.1962681	5.1962743	40.3122230	40.3121997	35.1159549	35.1159255
	0.0015691	0.0003146	-0.0000063	-0.0000012	0.0000233	0.0000006	0.0000295	0.0000008
4800.00	4.9960817	4.9946897	5.1920023	5.1919759	40.4173114	40.4172548	35.2253091	35.2252789
	0.0013919	0.0002786	0.0000264	0.0000051	0.0000566	0.0000014	0.0000302	0.0000009
4900.00	5.0059449	5.0048605	5.1881027	5.1880521	40.5204267	40.5203449	35.3323240	35.3322928
	0.0010844	0.0002166	0.0000506	0.0000098	0.0000819	0.0000020	0.0000312	0.0000009
5000.00	5.0164955	5.0158267	5.1845655	5.1844966	40.6216671	40.6215657	35.4371015	35.4370691
	0.0006687	0.0001333	0.0000689	0.0000133	0.0001014	0.0000025	0.0000324	0.0000009
5100.00	5.0277036	5.0275392	5.1813784	5.1813030	40.7211166	40.7210066	35.5397382	35.5397036
	0.0001644	0.0000327	0.0000753	0.0000145	0.0001100	0.0000027	0.0000346	0.0000010
5200.00	5.0395491	5.0399376	5.1785355	5.1784642	40.8188581	40.8187508	35.6403226	35.6402866
	-0.0003886	-0.0000771	0.0000713	0.0000138	0.0001073	0.0000026	0.0000360	0.0000010
5300.00	5.0520177	5.0529496	5.1760302	5.1759723	40.9149710	40.9148751	35.7389408	35.7389028
	-0.0009319	-0.0001845	0.0000578	0.0000112	0.0000959	0.0000023	0.0000381	0.0000011
5400.00	5.0650799	5.0664895	5.1738529	5.1738188	41.0095223	41.0094509	35.8356694	35.8356321
	-0.0014095	-0.0002783	0.0000341	0.0000066	0.0000714	0.0000017	0.0000373	0.0000010
5500.00	5.0787232	5.0804571	5.1719980	5.1719937	41.1025859	41.1025438	35.9305878	35.9305501
	-0.0017339	-0.0003414	0.0000043	0.0000008	0.0000421	0.0000010	0.0000378	0.0000011
5600.00	5.0929281	5.0947372	5.1704597	5.1704863	41.1942248	41.1942139	36.0237651	36.0237277
	-0.0018091	-0.0003552	-0.0000265	-0.0000051	0.0000109	0.0000003	0.0000374	0.0000010
5700.00	5.1076726	5.1091983	5.1692276	5.1692840	41.2844981	41.2845161	36.1152705	36.1152320
	-0.0015257	-0.0002987	-0.0000564	-0.0000109	-0.0000180	-0.0000004	0.0000385	0.0000011
5800.00	5.1229418	5.1236919	5.1682978	5.1683731	41.3734610	41.3734997	36.2051633	36.2051266
	-0.0007501	-0.0001464	-0.0000753	-0.0000146	-0.0000386	-0.0000009	0.0000367	0.0000010
5900.00	5.1387049	5.1380521	5.1676607	5.1677378	41.4611648	41.4612090	36.2935041	36.2934712
	0.0006528	0.0001270	-0.0000771	-0.0000149	-0.0000442	-0.0000011	0.0000329	0.0000009
6000.00	5.1549559	5.1520945	5.1673117	5.1673606	41.5476667	41.5476831	36.3803551	36.3803225
	0.0028614	0.0005551	-0.0000490	-0.0000095	-0.0000164	-0.0000004	0.0000326	0.0000009

MAX REL ERR CP/R = 0.000603 TEMP = 1100. AVER REL ERR CP/R = 0.000259 REL LST SQ ERR CP/R = 0.000298
MAX REL ERR HH/RT = 0.000075 TEMP = 1200. AVER REL ERR HH/RT = 0.000023 REL LST SQ ERR HH/RT = 0.000029
MAX REL ERR S/R = 0.000009 TEMP = 1500. AVER REL ERR S/R = 0.000003 REL LST SQ ERR S/R = 0.000004
MAX REL ERR GH/RT = 0.000006 TEMP = 1000. AVER REL ERR GH/RT = 0.000002 REL LST SQ ERR GH/RT = 0.000002
MAX ERR CP/R = 0.003958 TEMP = 1100. AVER ERR CP/R = 0.001377 LST SQ ERR CP/R = 0.001623
MAX ERR HH/RT = 0.000387 TEMP = 1200. AVER ERR HH/RT = 0.000123 LST SQ ERR HH/RT = 0.000155
MAX ERR S/R = 0.000302 TEMP = 1500. AVER ERR S/R = 0.000119 LST SQ ERR S/R = 0.000144
MAX ERR GH/RT = 0.000157 TEMP = 1000. AVER ERR GH/RT = 0.000059 LST SQ ERR GH/RT = 0.000067

CP/R = -1.3876702e+07T**-2.0 3.3903403e+04T**-1.0 -2.1906072e+01T** 0.0 1.0456393e-02T** 1.0 -2.2225473e-06T** 2.0
2.4662915e-10T** 3.0 -1.0961026e-14T** 4.0

(H-H0)/R CONSTANT = -0.22586827e+06, H/R CONSTANT =-0.21994504e+06, S/R CONSTANT = 0.20063928e+03

BAR MGO

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

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MGO              Magnesium Oxide.  JANAF Dec.1974, p1472.          Expl. 7
 2 J12/74 MG  1.000   1.00     0.00     0.00     0.00 0      40.30440      58158.000
    200.000  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8909.226
  3.77823092d+05 -6.08173235d+03  4.16158227d+01 -1.18519891d-01  1.94341613d-04
 -1.45495255d-07  4.03517625d-11  0.00000000d+00  3.43248026d+04 -2.01828144d+02
   1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0            8909.226
 -1.38767024d+07  3.39034027d+04 -2.19060721d+01  1.04563934d-02 -2.22254732d-06
  2.46629150d-10 -1.09610259d-14  0.00000000d+00 -2.19945038d+05  2.00639280d+02
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ORIGINAL BAR MGO

ORIGINAL MGO

	T DEG-K	CP J/MOL-K	H-H298 KJ/MOL	S J/MOL-K	-(G-H298)/T J/MOL-K	H KJ/MOL	DELTA H KJ/MOL	LOG K
	0	-------	-8.909	-------	-------	49.249	58.587	-------
	100	29.125	-6.001	180.487	240.496	52.157	59.403	-26.6232
	200	30.117	-3.054	200.876	216.146	55.104	58.887	-11.1490
	298.15	32.174	0.000	213.272	213.272	58.158	58.158	-6.1132
	300	32.215	0.060	213.471	213.273	58.218	58.144	-6.0503
	400	34.783	3.403	223.072	214.565	61.561	57.447	-3.5336
	500	38.435	7.053	231.203	217.096	65.211	56.901	-2.0403
	600	43.079	11.124	238.611	220.071	69.282	56.624	-1.0523
	700	47.786	15.671	245.612	223.224	73.829	56.672	-0.3482
	800	51.561	20.650	252.254	226.442	78.808	56.993	0.1817
	900	53.891	25.935	258.476	229.660	84.093	57.457	0.5968
*	1000	54.796	31.380	264.212	232.832	89.538	49.314	0.8943
	1100	54.609	36.857	269.433	235.926	95.015	49.605	1.1292
	1200	53.730	42.279	274.151	238.918	100.437	49.821	1.3259
	1300	52.496	47.592	278.404	241.795	105.750	49.910	1.4929
	1400	51.140	52.774	282.245	244.549	110.932	49.854	1.6361
	1500	49.802	57.820	285.727	247.180	115.978	49.648	1.7599
	1600	48.558	62.737	288.901	249.690	120.895	49.299	1.8676
	1700	47.439	67.536	291.811	252.084	125.694	48.820	1.9618
	1800	46.455	72.230	294.494	254.366	130.388	48.223	2.0447
	1900	45.599	76.831	296.982	256.544	134.989	47.523	2.1178
	2000	44.862	81.354	299.302	258.625	139.512	46.731	2.1826
	2100	44.231	85.807	301.475	260.614	143.965	45.859	2.2402
	2200	43.691	90.203	303.520	262.518	148.361	44.917	2.2915
	2300	43.232	94.548	305.451	264.343	152.706	43.913	2.3374
	2400	42.841	98.851	307.283	266.095	157.009	42.856	2.3785
	2500	42.510	103.118	309.025	267.777	161.276	41.752	2.4153
	2600	42.230	107.355	310.686	269.396	165.513	40.606	2.4484
	2700	41.993	111.566	312.276	270.955	169.724	39.423	2.4782
	2800	41.795	115.755	313.799	272.458	173.913	38.207	2.5050
	2900	41.630	119.926	315.263	273.909	178.084	36.963	2.5292
	3000	41.493	124.082	316.672	275.311	182.240	35.694	2.5510
	3100	41.381	128.225	318.030	276.667	186.383	34.403	2.5707
	3200	41.291	132.359	319.343	277.981	190.517	33.091	2.5885
	3300	41.221	136.484	320.612	279.253	194.642	31.763	2.6045
	3400	41.167	140.604	321.842	280.488	198.762	30.418	2.6190
	3500	41.129	144.718	323.035	281.687	202.876	29.061	2.6321
	3600	41.104	148.830	324.193	282.851	206.988	27.692	2.6438
	3700	41.091	152.940	325.319	283.984	211.098	26.312	2.6544
	3800	41.090	157.049	326.415	285.086	215.207	24.925	2.6639
	3900	41.099	161.158	327.482	286.160	219.316	23.529	2.6725
	4000	41.117	165.269	328.523	287.206	223.427	22.127	2.6801
	4100	41.144	169.382	329.539	288.226	227.540	20.720	2.6869
	4200	41.180	173.498	330.530	289.221	231.656	19.310	2.6930
	4300	41.223	177.618	331.500	290.193	235.776	17.896	2.6984
	4400	41.273	181.743	332.448	291.143	239.901	16.480	2.7031
	4500	41.330	185.873	333.376	292.071	244.031	15.063	2.7073
	4600	41.394	190.009	334.285	292.979	248.167	13.645	2.7109
	4700	41.464	194.152	335.176	293.868	252.310	12.228	2.7140
	4800	41.540	198.302	336.050	294.737	256.460	10.812	2.7167
	4900	41.622	202.460	336.907	295.589	260.618	9.398	2.7190
	5000	41.710	206.626	337.749	296.424	264.784	7.987	2.7208
	5100	41.803	210.802	338.576	297.242	268.960	6.578	2.7223
	5200	41.901	214.987	339.389	298.045	273.145	5.175	2.7235
	5300	42.005	219.182	340.188	298.833	277.340	3.776	2.7243
	5400	42.114	223.388	340.974	299.606	281.546	2.382	2.7249
	5500	42.227	227.605	341.748	300.365	285.763	0.995	2.7252
	5600	42.345	231.834	342.510	301.111	289.992	-0.386	2.7252
	5700	42.468	236.074	343.260	301.844	294.232	-1.759	2.7251
	5800	42.595	240.328	344.000	302.564	298.486	-3.124	2.7247
	5900	42.726	244.594	344.729	303.273	302.752	-4.480	2.7241
	6000	42.861	248.873	345.448	303.970	307.031	-5.827	2.7233

*A CHANGE IN PHASE OF AN ASSIGNED REFERENCE ELEMENT HAS OCCURRED BETWEEN THIS TEMPERATURE AND THE PRECEDING ONE,
MG-- 923.000

COEFFICIENTS MGO

	T DEG-K	CP J/MOL-K	H-H298 KJ/MOL	S J/MOL-K	-(G-H298)/T J/MOL-K	H KJ/MOL	DELTA H KJ/MOL	LOG K
	0	-------	-8.909	-------	-------	49.249	58.587	-------
	200	30.124	-3.048	200.900	216.141	55.110	58.893	-11.1492
	298.15	32.174	0.000	213.272	213.272	58.158	58.158	-6.1132
	300	32.216	0.060	213.471	213.273	58.218	58.144	-6.0503
	400	34.762	3.402	223.069	214.564	61.560	57.446	-3.5336
	500	38.448	7.052	231.199	217.095	65.210	56.899	-2.0403
	600	43.092	11.124	238.611	220.070	69.282	56.625	-1.0524
	700	47.773	15.671	245.611	223.223	73.829	56.672	-0.3482
	800	51.560	20.649	252.251	226.441	78.807	56.993	0.1817
	900	53.898	25.935	258.475	229.658	84.093	57.456	0.5967
*	1000	54.794	31.379	264.210	232.831	89.537	49.314	0.8942
	1200	53.719	42.282	274.153	238.918	100.440	49.824	1.3258
	1400	51.118	52.773	282.243	244.549	110.931	49.853	1.6361
	1600	48.572	62.736	288.899	249.689	120.894	49.297	1.8675
	1800	46.478	72.232	294.494	254.365	130.390	48.226	2.0446
	2000	44.871	81.359	299.304	258.624	139.517	46.737	2.1826
	2200	43.682	90.208	303.522	262.518	148.366	44.922	2.2915
	2400	42.823	98.854	307.284	266.094	157.012	42.859	2.3785
	2600	42.213	107.354	310.686	269.396	165.512	40.605	2.4484
	2800	41.786	115.752	313.798	272.458	173.910	38.204	2.5050
	3000	41.494	124.078	316.670	275.311	182.236	35.690	2.5510

*A CHANGE IN PHASE OF AN ASSIGNED REFERENCE ELEMENT HAS OCCURRED BETWEEN THIS TEMPERATURE AND THE PRECEDING ONE,
MG-- 923.000

COEFFICIENTS BAR MGO

Example 8 (Na_2CO_3(1,2,ℓ) by Methods READIN and COEF with LSQS and LOGK Options)

Problem.—Calculate thermodynamic properties for a condensed species with more than two phases. Use different methods for processing the data, if needed. Obtain least-squares coefficients and tables with $\Delta_f H^o_T$ and $\log_{10}K$ columns.

The species selected for this example is Na_2CO_3 which has three condensed phases—two solid and one liquid. This example illustrates the following features:

(1) The NAME records identify the three phases as Na_2CO_3(1), Na_2CO_3(2), and Na_2CO_3(ℓ). These names appear as identification in the least-squares coefficient output.

(2) The data for the two solid phases are processed by METHOD READIN, while the liquid phase is processed by METHOD COEF. The energy unit for input data is in calories as indicated by the CAL label on the METHOD records.

(3) The heat of formation at 298.15 K is specified to be −270.26 kcal/mol by HF298 and KCAL on the formula record.

(4) The OUTP record contains the labels LOGK, JOULES, and LSQS. The LSQS label calls for output tables of functions calculated from least-squares coefficients. Separate sets of coefficients will be generated for each phase. The LOGK label calls for tables of rounded functions including $\Delta_f H^o_T$ and $\log_{10}K$. The label JOULES specifies that the unit of energy in the output tables is in joules.

(5) The first METHOD record specifies that the energy unit on the input data records following it is in calories (CAL). (Note that while the input is in calories the output, as discussed in (4) above, is to be in joules.)

(6) The heat of transition between the first and second phase is given by the value of 165. for the DELTAH label on the second METHOD record. The energy unit is cal/mol (CAL).

(7) No enthalpy or entropy values are given on the first data record for the second phase at the transition temperature of 723.15 K. These values are calculated by the program from the DELTAH value of 165 cal/mol and the enthalpy and entropy values of the first phase at 723.15 K.

(8) The heat of transition of 7090. between phases 2 and 3 (the heat of fusion) is given on the third METHOD record as the DELTAH numerical value. The energy unit is cal/mol (CAL).

(9) On the first data record for the liquid phase, C1 is given as 45.30.

(10) On the second data record for the liquid phase, only the TCOEF label appears. The purpose of the TCOEF label was discussed in the example for Mg(ℓ).

(11) The listed output consists of a table of the input records, a table of least-squares coefficients and errors, and a table of rounded thermodynamic functions. Note that at each transition temperature (T = 723.15 and 1123.15 K) values of −(G-H298)/T and LOGK are identical for the two phases. The columns headed DELTA H and LOGK do not contain data for temperatures at 2400 K and higher, inasmuch as the EF data for Na(ℓ) exist only to 2300 K.

Input. - The input data set for $Na_2CO_3(1,2,\ell)$, example 8, is as follows:

	Rec. ID 1-6	Label 1 7-12	Numerical value 1 13-24	Label 2 25-30	Numerical value 2 31-42	Label 3 43-48	Numerical value 3 49-60	Label 4 61-66	Numerical value 4 67-78	79-80
a	NAME	NA2CO3(1)		JANAF	DATA. MARCH	1966.			Expl.	8
a	NAME	NA2CO3(2)		JANAF	DATA. MARCH	1966.				
a	NAME	NA2CO3(L)		JANAF	DATA. MARCH	1966.				
	NA2CO3(S)			HF298	-270.26	KCAL				
	DATE	J 3/66								
	OUTP	LOGK		JOULES		LSQS				
	METHOD	READIN		H298H0	4974.	MELTPT	1123.15	CAL		
		T	100.	CP	14.637	S	10.334	H-H2	-4348.	
		T	200.	CP	22.5000	S	23.367	H-H2	-2424.	
		T	298.15	CP	26.530	S	33.173	H-H2	0.0	
		T	300.	CP	26.590	S	33.338	H-H2	49.0	
		T	400.	CP	29.900	S	41.421	H-H2	2867.	
		T	500.	CP	33.990	S	48.520	H-H2	6056.	
		T	600.	CP	39.030	S	55.153	H-H2	9702.	
		T	700.	CP	44.830	S	61.597	H-H2	13890.	
		T	723.15	CP	46.220	S	63.078	H-H2	14944.	
	METHOD	READIN		DELTAH	165.	CAL				
		T	723.15	CP	34.360	S		H-H2		
		T	800.	CP	36.650	S	66.889	H-H2	17837.	
		T	900.	CP	39.730	S	71.383	H-H2	21655.	
		T	1000.	CP	42.830	S	75.729	H-H2	25782.	
		T	1100.	CP	45.900	S	79.956	H-H2	30220.	
		T	1123.15	CP	46.630	S	80.920	H-H2	31291.	
	TEMP	T	1123.15	T	1200.	I	200.	T	6000.	
	METH	COEF		DELTAH	7090.0	CAL				
		T	1123.15	T	6000.	C1	45.30	E1	0.0	
		TCOEF								
	FINISH									

[a]All alphanumeric characters.

Listed output. - Listed output for $Na_2CO_3(1,2,\ell)$, example, 8, is as follows:

```
NAME  NA2CO3(1)          JANAF DATA.  MARCH 1966.                          Expl. 8
NAME  NA2CO3(2)          JANAF DATA.  MARCH 1966.
NAME  NA2CO3(L)          JANAF DATA.  MARCH 1966.
NA2C1O3(S)               HF298 -270.26     KCAL
DATE  J 3/66
OUTP  LOGK               JOULES            LSQS
METHODREADIN             H298H0 4974.      MELTPT  1123.15   CAL
      T     100.         CP    14.637      S       10.334      H-H2  -4348.
      T     200.         CP    22.5000     S       23.367      H-H2  -2424.
      T     298.15       CP    26.530      S       33.173      H-H2  0.0
      T     300.         CP    26.590      S       33.338      H-H2  49.0
      T     400.         CP    29.900      S       41.421      H-H2  2867.
      T     500.         CP    33.990      S       48.520      H-H2  6056.
      T     600.         CP    39.030      S       55.153      H-H2  9702.
      T     700.         CP    44.830      S       61.597      H-H2  13890.
      T     723.15       CP    46.220      S       63.078      H-H2  14944.
METHODREADIN             DELTAH   165.     CAL
```

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
200.00	11.3223750	11.3218818	6.4160125	6.4142146	11.7586638	11.7561738	5.3426513	5.3419592
	0.0004931	0.0000436	0.0017979	0.0002802	0.0024900	0.0002118	0.0006921	0.0001295
298.15	13.3503381	13.3503381	8.3951021	8.3951021	16.6932065	16.6932065	8.2981043	8.2981043
	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
300.00	13.3805311	13.3807015	8.4255244	8.4257531	16.7762372	16.7758823	8.3507128	8.3501292
	-0.0001704	-0.0000127	-0.0002287	-0.0000271	0.0003549	0.0000212	0.0005836	0.0000699
400.00	15.0461783	15.0471258	9.8643047	9.8689109	20.8437375	20.8491163	10.9794328	10.9802053
	-0.0009475	-0.0000630	-0.0046062	-0.0004670	-0.0053787	-0.0002581	-0.0007725	-0.0000704
500.00	17.1043345	17.1006858	11.1009596	11.1014685	24.4160726	24.4179923	13.3151130	13.3165238
	0.0036487	0.0002133	-0.0005089	-0.0000458	-0.0019197	-0.0000786	-0.0014108	-0.0001060
600.00	19.6405465	19.6447778	12.3086796	12.3071219	27.7539088	27.7538865	15.4452291	15.4467646
	-0.0042313	-0.0002154	0.0015578	0.0001266	0.0000223	0.0000008	-0.0015355	-0.0000994
700.00	22.5592031	22.5547150	13.5609703	13.5599048	30.9966370	30.9970958	17.4356667	17.4371910
	0.0044881	0.0001989	0.0010655	0.0000786	-0.0004588	-0.0000148	-0.0015243	-0.0000874
723.15	23.2586743	23.2615218	13.8602912	13.8591431	31.7419008	31.7423558	17.8816097	17.8832127
	-0.0028475	-0.0001224	0.0011481	0.0000828	-0.0004549	-0.0000143	-0.0016030	-0.0000896

```
  MAX REL ERR CP/R  =  0.000215    TEMP =   600.      AVER REL ERR CP/R  =  0.000109      REL LST SQ ERR CP/R  =  0.000138
  MAX REL ERR HH/RT =  0.000467    TEMP =   400.      AVER REL ERR HH/RT =  0.000139      REL LST SQ ERR HH/RT =  0.000203
  MAX REL ERR S/R   =  0.000258    TEMP =   400.      AVER REL ERR S/R   =  0.000075      REL LST SQ ERR S/R   =  0.000122
  MAX REL ERR GH/RT =  0.000130    TEMP =   200.      AVER REL ERR GH/RT =  0.000082      REL LST SQ ERR GH/RT =  0.000089
      MAX ERR CP/R  =  0.004488    TEMP =   700.         AVER ERR CP/R  =  0.002103          LST SQ ERR CP/R  =  0.002753
      MAX ERR HH/RT =  0.004606    TEMP =   400.         AVER ERR HH/RT =  0.001364          LST SQ ERR HH/RT =  0.001925
      MAX ERR S/R   =  0.005379    TEMP =   400.         AVER ERR S/R   =  0.001385          LST SQ ERR S/R   =  0.002218
      MAX ERR GH/RT =  0.001603    TEMP =   723.         AVER ERR GH/RT =  0.001015          LST SQ ERR GH/RT =  0.001154
CP/R =    2.7690834e+05T**-2.0  -6.2925704e+03T**-1.0   5.4857058e+01T** 0.0  -1.3550634e-01T** 1.0   2.3061993e-04T** 2.0
        -1.4673680e-07T** 3.0   3.4582744e-11T** 4.0
(H-H0)/R CONSTANT =  0.27187630e+05, H/R CONSTANT =-0.11131471e+06, S/R CONSTANT =-0.28402909e+03
```

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

```
NA2CO3(1)          JANAF DATA.  MARCH 1966.                          Expl. 8
 1 J 3/66 NA  2.00C   1.000   3.00     0.00     0.00 1     105.98874    -1130767.840
   200.000   723.150 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          20811.216
 2.76908339d+05 -6.29257045d+03  5.48570580d+01 -1.35506338d-01  2.30619932d-04
-1.46736800d-07  3.45827436d-11  0.00000000d+00 -1.11314706d+05 -2.84029093d+02
```

```
      T     723.15       CP    34.360      S                   H-H2
      T     800.         CP    36.650      S       66.889      H-H2  17837.
      T     900.         CP    39.730      S       71.383      H-H2  21655.
                                          NA2CO3(1)         NA2CO3(2)         NA2CO3(L)
      T     1000.        CP    42.830      S       75.729      H-H2  25782.
      T     1100.        CP    45.900      S       79.956      H-H2  30220.
      T     1123.15      CP    46.630      S       80.920      H-H2  31291.
TEMP  T     1123.15      T     1200.       I       200.        T     6000.
METH  COEF               DELTAH7090.0      CAL
                                          NA2CO3(1)         NA2CO3(2)         NA2CO3(L)
```

LEAST SQUARES

T	CP/R INPUT INPUT-CALC	CP/R CALC FRACTION	HH/RT INPUT INPUT-CALC	HH/RT CALC FRACTION	S/R INPUT INPUT-CALC	S/R CALC FRACTION	-GH/RT INPUT INPUT-CALC	-GH/RT CALC FRACTION
723.15	17.2905246	17.2905246	13.9751093	13.9739612	31.8567190	31.8571739	17.8816097	17.8832127
	0.0000000	0.0000000	0.0011481	0.0000822	-0.0004549	-0.0000143	-0.0016030	-0.0000896
800.00	18.4428908	18.4427379	14.3485942	14.3478323	33.6596596	33.6605661	19.3110654	19.3127337
	0.0001529	0.0000083	0.0007619	0.0000531	-0.0009065	-0.0000269	-0.0016684	-0.0000864
900.00	19.9927981	19.9927417	14.8890629	14.8884219	35.9211153	35.9217548	21.0320524	21.0333330
	0.0000564	0.0000028	0.0006410	0.0000431	-0.0006396	-0.0000178	-0.0012806	-0.0000609
1000.00	21.5527698	21.5527326	15.4769318	15.4770866	38.1080949	38.1091833	22.6311631	22.6320967
	0.0000372	0.0000017	-0.0001548	-0.0000100	-0.0010885	-0.0000286	-0.0009336	-0.0000413
1100.00	23.0976450	23.0977521	16.1001885	16.0994725	40.2351917	40.2356566	24.1350032	24.1361841
	-0.0001071	-0.0000046	0.0007160	0.0000445	-0.0004648	-0.0000116	-0.0011808	-0.0000489
1123.15	23.4649931	23.4649481	16.2481880	16.2474895	40.7202926	40.7205117	24.4721046	24.4730222
	0.0000450	0.0000019	0.0006985	0.0000430	-0.0002191	-0.0000054	-0.0009176	-0.0000375

MAX REL ERR CP/R = 0.000008 TEMP = 800.
MAX REL ERR HH/RT = 0.000082 TEMP = 723.
MAX REL ERR S/R = 0.000029 TEMP = 1000.
MAX REL ERR GH/RT = 0.000090 TEMP = 723.
MAX ERR CP/R = 0.000153 TEMP = 800.
MAX ERR HH/RT = 0.001148 TEMP = 723.
MAX ERR S/R = 0.001088 TEMP = 1000.
MAX ERR GH/RT = 0.001668 TEMP = 800.

AVER REL ERR CP/R = 0.000003
AVER REL ERR HH/RT = 0.000046
AVER REL ERR S/R = 0.000017
AVER REL ERR GH/RT = 0.000061
AVER ERR CP/R = 0.000066
AVER ERR HH/RT = 0.000687
AVER ERR S/R = 0.000629
AVER ERR GH/RT = 0.001264

REL LST SQ ERR CP/R = 0.000004
REL LST SQ ERR HH/RT = 0.000051
REL LST SQ ERR S/R = 0.000019
REL LST SQ ERR GH/RT = 0.000064
LST SQ ERR CP/R = 0.000083
LST SQ ERR HH/RT = 0.000745
LST SQ ERR S/R = 0.000694
LST SQ ERR GH/RT = 0.001298

CP/R = -1.1212220e+08T**-2.0 6.4050666e+05T**-1.0 -1.4442432e+03T** 0.0 1.6431542e+00T** 1.0 -9.0577776e-04T** 2.0
2.0003499e-07T** 3.0

(H-H0)/R CONSTANT = -0.36465252e+07, H/R CONSTANT =-0.37850275e+07, S/R CONSTANT = 0.93420894e+04

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

```
NA2CO3(2)         JANAF DATA.  MARCH 1966.
 1 J 3/66 NA  2.00C   1.000   3.00    0.00    0.00 2    105.98874   -1130767.840
   723.150  1123.150 6 -2.0 -1.0  0.0  1.0  2.0  3.0  0.0  0.0         20811.216
-1.12122199d+08  6.40506661d+05 -1.44424316d+03  1.64315419d+00 -9.05777755d-04
 2.00034993d-07  0.00000000d+00  0.00000000d+00 -3.78502749d+06  9.34208940d+03

      T     1123.15     T     6000.       C1    45.30       E1    0.0

      TCOEF

FINISH
```

COEFFICIENTS ADJUSTED TO FIT UPPER PHASE AT 1123.15

NA2CO3(1) NA2CO3(2) NA2CO3(L)

THERMODYNAMIC DATA COEFFICIENTS, RECORD IMAGES -

```
NA2CO3(L)         JANAF DATA.  MARCH 1966.
 1 J 3/66 NA  2.00C   1.000   3.00    0.00    0.00 3    105.98874   -1130767.840
   1123.150  6000.000 1  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0         20811.216
 2.27957150d+01  0.00000000d+00  0.00000000d+00  0.00000000d+00  0.00000000d+00
 0.00000000d+00  0.00000000d+00  0.00000000d+00 -1.42289169d+05 -1.16217533d+02
```

ORIGINAL NA2CO3(1) NA2CO3(2) NA2CO3(L)

ORIGINAL NA2CO3(1) NA2CO3(2) NA2CO3(L)

	T DEG-K	CP J/MOL-K	H-H298 KJ/MOL	S J/MOL-K	-(G-H298)/T J/MOL-K	H KJ/MOL	DELTA H KJ/MOL	LOG K
	0	-------	-20.811	-------	-------	-1151.579	-1124.585	-------
	100	61.241	-18.192	43.237	225.158	-1148.960	-1129.073	575.9119
	200	94.140	-10.142	97.768	148.478	-1140.910	-1130.627	280.8333
	298.15	111.002	0.000	138.796	138.796	-1130.768	-1130.768	183.6185
	300	111.253	0.205	139.486	138.803	-1130.563	-1130.765	182.3971
*	400	125.102	11.996	173.305	143.317	-1118.772	-1135.691	133.1291
	500	142.214	25.338	203.008	152.331	-1105.430	-1134.481	103.4801
	600	163.302	40.593	230.760	163.105	-1090.175	-1131.600	83.7484
	700	187.569	58.116	257.722	174.699	-1072.652	-1126.656	69.7019
	723.15	193.384	62.526	263.918	177.455	-1068.242	-1125.185	67.0121
	723.15	143.762	63.216	264.873	177.455	-1067.552	-1124.494	67.0121
	800	153.344	74.630	279.864	186.576	-1056.138	-1122.900	59.2148
	900	166.230	90.605	298.666	197.995	-1040.163	-1119.841	51.0787
	1000	179.201	107.872	316.850	208.978	-1022.896	-1115.648	44.5907
	1100	192.046	126.440	334.536	219.590	-1004.327	-1110.316	39.3048
	1123.15	195.100	130.922	338.569	222.003	-999.846	-1108.925	38.2188
	1123.15	189.535	160.586	364.981	222.003	-970.182	-1079.260	38.2188
	1200	189.535	175.152	377.525	231.566	-955.616	-1075.023	35.0107
	1400	189.535	213.059	406.742	254.558	-917.709	-1064.586	28.3572
	1600	189.535	250.966	432.051	275.198	-879.802	-1055.196	23.4137
	1800	189.535	288.873	454.375	293.890	-841.895	-1047.130	19.6006
	2000	189.535	326.780	474.345	310.955	-803.988	-1040.691	16.5716
	2200	189.535	364.687	492.410	326.643	-766.081	-1036.189	14.1062
	2400	189.535	402.594	508.901	341.154	-728.174		
	2600	189.535	440.501	524.072	354.649	-690.267		
	2800	189.535	478.408	538.118	367.258	-652.360		
	3000	189.535	516.315	551.195	379.090	-614.453		
	3200	189.535	554.222	563.427	390.233	-576.546		
	3400	189.535	592.129	574.918	400.762	-538.639		
	3600	189.535	630.036	585.751	410.741	-500.731		
	3800	189.535	667.943	595.999	420.224	-462.824		
	4000	189.535	705.850	605.721	429.258	-424.917		
	4200	189.535	743.757	614.968	437.883	-387.010		
	4400	189.535	781.665	623.785	446.134	-349.103		
	4600	189.535	819.572	632.211	454.043	-311.196		
	4800	189.535	857.479	640.277	461.636	-273.289		
	5000	189.535	895.386	648.014	468.937	-235.382		
	5200	189.535	933.293	655.448	475.969	-197.475		
	5400	189.535	971.200	662.601	482.749	-159.568		
	5600	189.535	1009.107	669.494	489.296	-121.661		
	5800	189.535	1047.014	676.145	495.625	-83.754		
	6000	189.535	1084.921	682.571	501.750	-45.847		

*A CHANGE IN PHASE OF AN ASSIGNED REFERENCE ELEMENT HAS OCCURRED BETWEEN THIS TEMPERATURE AND THE PRECEDING ONE,
NA-- 371.010

ORIGINAL NA2CO3(1) NA2CO3(2) NA2CO3(L)

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TABLE I. - FILL PROCEDURE PARAMETERS

Atomic number	Chemical symbol	$\sum_i g_i$	b (or c*)	Atomic number	Chemical symbol	$\sum_i g_i$	b (or c*)
1	H	2	2	38	Sr	670	4
2	He	1	4	39	Y	1260	[a]1170
3	Li	8	2	40	Zr	3855	[a]3780
4	Be	13	4	41	Nb	7992	[a]8100
5	B	6	2	42	Mo	11676	[a]12096
6	C	15	12	43	Te	12216	[a]12852
7	N	20	30	44	Ru	9135	[a]9720
8	O	15	40	45	Rh	4780	[a]5130
9	F	6	30	46	Pd	1666	[a]1800
10	Ne	1	12	47	Ag	394	2
11	Na	18	2	48	Cd	125	4
12	Mg	33	4	49	In	92	2
13	Al	16	2	50	Sn	351	12
14	Si	75	12	51	Sb	860	30
15	P	170	30	52	Te	1135	40
16	S	215	40	53	I	846	30
17	Cl	156	30	54	Xe	337	12
18	Ar	61	12	55	Cs	124	2
19	K	42	2	56	Ba	1138	4
20	Ca	426	4	57	La	2200	[a]1170
21	Sc	1260	[a]1170	Lanthanide series-4f shell filled			
22	Ti	3855	[a]3780	72	Hf	3855	[a]3780
23	V	7992	[a]8100	73	Ta	7992	[a]8100
24	Cr	11676	[a]12096	74	W	11676	[a]12096
25	Mn	12216	[a]12852	75	Re	12216	[a]12852
26	Fe	9135	[a]9720	76	Os	9135	[a]9720
27	Co	4780	[a]5130	77	Ir	4780	[a]5130
28	Ni	1666	[a]1800	78	Pt	1666	[a]1800
29	Cu	362	2	79	Au	434	2
30	Zn	61	4	80	Hg	205	4
31	Ga	30	2	81	Tl	132	2
32	Ge	159	12	82	Pb	591	12
33	As	380	30	83	Bi	1460	30
34	Se	495	40	84	Po	1935	40
35	Br	366	30	85	At	1446	30
36	Kr	145	12	86	Rn	577	12
37	Rb	74	2				

[a]This is the c* value which represents the total quantum weight for each value of n above the ground state principal quantum number. In BLOCK DATA, these values are given as negative values in order for the PAC91 program to differentiate the b values from the c* values.

TABLE II. - SOME TERMS IN ln Q AND THEIR DERIVATIVES

Formula number	Method				Subscript in equation (9)	$\ln Q^m$ terms	$T\frac{d(\ln Q^m)}{dT}$ terms	$T^2\frac{d^2(\ln Q^m)}{dT^2}$ terms	Remarks			
	RRHO[a]	PANDK[b] and JANAF[c]	NRRAO1[d]	NRRAO2[e]					Type of molecule			Definitions
									Diatomic	Linear polyatomic	Nonlinear	
1	Yes	Yes	Yes	Yes	e	$\ln g_m - \frac{c_2 T_0}{T}$	$\frac{c_2 T_0}{T}$	$\frac{-2c_2 T_0}{T}$	Yes	Yes	Yes	$c_2 = hc/k$ g_m = statistical weight T_0 = electronic excitation energy
2	Yes	Yes	Yes	Yes	V	$\sum_{i=1}^{n} d_i \ln(s_i)$	$\sum_{i=1}^{n} d_i u_i r_i s_i$	$\sum_{i=1}^{n} d_i u_i r_i s_i (u_i s_i - 2)$	Yes	Yes	Yes	d_i = degeneracy n = number of unique frequencies $u_i = c_2\nu_i/T$ $r_i = e^{-u_i}$ $s_i = 1/(1 - r_i)$
									Yes	No	No	$\nu_1 = \omega_e - 2\omega_e x_e + 3.25\omega_e y_e + 5\omega_e z_e$
3	Yes	Yes	Yes	Yes	R	For diatomic and linear molecules, $-\ln\frac{c_2 B_0 \sigma}{T}$	1	-1	Yes	Yes	Yes	σ = symmetry number
									Yes	Yes	No	$B_0 = B_e - \frac{\alpha_1}{2} + \frac{\alpha_2}{4} + \frac{\alpha_3}{8}$
4	Yes	Yes	Yes	Yes	R	For nonlinear molecules, $\frac{1}{2}\ln\left[\frac{\pi}{\sigma^2 A_0 B_0 C_0}\left(\frac{T}{c_2}\right)^3\right]$	3/2	-3/2	No	No	Yes	$A_0 = A_e - \frac{1}{2}\sum_{i=1}^{n} d_i \alpha_i^A$
									No	No	Yes	$B_0 = B_e - \frac{1}{2}\sum_{i=1}^{n} d_i \alpha_i^B$
									No	No	Yes	$C_0 = C_e - \frac{1}{2}\sum_{i=1}^{n} d_i \alpha_i^C$
5	No	Yes	No	No	ρ	For JANAF only, ρT	ρT	0	Yes	Yes	No	This line for JANAF only; $\rho = 4\left(\frac{D_0}{B_e}\right)^{1/2} \Big/ \nu_1 c_2$
5a	No	Yes	Yes	Yes	ρ	For diatomic and linear polyatomic,			Yes	Yes	No	ρ is given or $\rho = \frac{D_0}{c_2 B_0^2}$ (except for JANAF)
						$2\rho T + 10\rho^2 T^2 + \frac{296\rho^3 T^3}{3} - \frac{2D_0}{3B_0}$	$2\rho T + 20\rho^2 T^2 + 296\rho^3 T^3$	$20\rho^2 T^2 + 592\rho^3 T^3$	Yes	No	No	$D_0 = D_e - \frac{\beta_1}{2} + \frac{\beta_2}{4} + \frac{\beta_3}{8}$; if not given, $D_e = \frac{4B_e^3}{\omega_e^2}$
									No	Yes	No	$D_0 = D_{000}$

TABLE II. - Continued.

Formula number	Method				Subscript in equation (9)	$\ln Q^m$ terms	$T\frac{d(\ln Q^m)}{dT}$ terms	$T^2\frac{d^2(\ln Q^m)}{dT^2}$ terms	Remarks			
	RRHO[a]	PANDK[b] and JANAF[c]	NRRAO1[d]	NRRAO2[e]					Type of molecule			Definitions
									Diatomic	Linear polyatomic	Nonlinear	
5b	No	Yes	Yes	Yes	ρ	For spherical top, $\frac{s}{16} + \frac{15\rho T}{4} + \frac{45\rho^2T^2}{2} + \frac{1035\rho^3T^3}{4} + \frac{16875\rho^4T^4}{4} - \frac{3D_0}{4B_0}$	$\frac{-s}{16} + \frac{15\rho T}{4} + 45\rho^2T^2 + \frac{3105\rho^3T^3}{4} + 16875\rho^4T^4$	$\frac{s}{8} + 45\rho^2T^2 + \frac{3105\rho^3T^3}{2} + 50625\rho^4T^4$	No	No	Yes	Spherical top only $s = c_2D_0/T$ $\rho = D_0/C_2B_0^2$
5c	No	Yes	Yes	Yes	ρ	For symmetrical top, $\rho_1T + \frac{(2\rho_2 - \rho_1^2)}{2}T^2$	$\rho_1T + (2\rho_2 - \rho_1^2)T^2$	$(2\rho_2 - \rho_1^2)T^2$	No	No	Yes	Symmetrical top only (see * for definition of ρ_1 and ρ_2)
5d	No	Yes	Yes	Yes	ρ	For asymmetrical top, ρT	ρT	0	No	No	Yes	Asymmetrical top only (see *** for definition of ρ for asymmetrical top)
6	No	Yes	Yes	Yes	Θ	$\ln\left(1 + \frac{\Theta_1}{T} + \frac{\Theta_2}{T^2} + \frac{\Theta_3}{T^3}\right)$	$-\left(\frac{\Theta_1}{T} + \frac{2\Theta_2}{T^2} + \frac{3\Theta_3}{T^3}\right)\frac{1}{Q_\Theta}$	$\left(\frac{2\Theta_1}{T} + \frac{6\Theta_2}{T^2} + \frac{12\Theta_3}{T^3}\right)\frac{1}{Q_\Theta} - \left[T\frac{d(\ln Q_\Theta)}{dT}\right]^2$	Yes	Yes	No	$\Theta_1 = \frac{c_2B_0}{3}$, $\Theta_2 = \frac{(c_2B_0)^2}{15}$, $\Theta_3 = \frac{4(c_2B_0)^3}{315}$
									No	No	Yes	$\Theta_1 = \frac{c_2}{12}\left[2(A_0 + B_0 + C_0) - \frac{A_0B_0}{C_0} - \frac{A_0C_0}{B_0} - \frac{B_0C_0}{A_0}\right]$
									No	No	Yes	$\Theta_2 = \frac{c_2^2}{480}\left[10(A_0^2 + B_0^2 + C_0^2) + 12(A_0B_0 + A_0C_0 + B_0C_0) - 12\left(\frac{A_0^2B_0 + A_0B_0^2}{C_0} + \frac{B_0^2C_0 + B_0C_0^2}{A_0} + \frac{A_0^2C_0 + A_0C_0^2}{B_0}\right) + 7\left(\frac{A_0^2B_0^2}{C_0^2} + \frac{A_0^2C_0^2}{B_0^2} + \frac{B_0^2C_0^2}{A_0^2}\right)\right]$
									No	No	Yes	$\Theta_3 = 0$

TABLE II. - Concluded.

Formula number	Method				Subscript in equation (9)	$\ln Q^m$ terms	$T\frac{d(\ln Q^m)}{dT}$ terms	$T^2\frac{d^2(\ln Q^m)}{dT^2}$ terms	Remarks			
	RRHO[a]	PANDK[b] and JANAF[c]	NRRAO1[d]	NRRAO2[e]					Type of molecule			Definitions
									Diatomic	Linear polyatomic	Nonlinear	
7	No	No	Yes	Yes	W	Triatomic linear molecules where Fermi resonance occurs $\left(\frac{c_2}{T}\right)^2\frac{W_0^2}{2}r_W s_W^2 s_2^2(1 - r_1)$	$\ln Q_W\left(S - \frac{r_1u_1}{1 - r_1}\right)$	$\ln Q_W\left[2u_W^2 r_W s_W(1 + r_W s_W) + 2u_2^2 r_2 s_2(1 + r_2 s_2) + S^2 - 2S - 2 - \frac{r_1u_1(u_1 + 2S - 2)}{1 - r_1}\right]$	No	Yes	No	W_0 = Fermi resonance constant $u_W = 2c_2\nu_2/T$ $r_W = e^{-u_W}$ $s_W = 1/(1 - r_W)$ $S = (1 + 2r_W s_W)u_W + 2(r_2u_2s_2 - 1)$

[a]Rigid-Rotator Harmonic-Oscillator approximation.
[b]Modified Pennington and Kobe method.
[c]Joint Army Navy Air Force method.
[d]Nonrigid-Rotator Anharmonic-Oscillator 1.
[e]Nonrigid-Rotator Anharmonic-Oscillator 2.

*For symmetrical top molecules, (see ref. 8)

$$\rho_1 = \frac{1}{4c_2B_0^2}\left[(8 + 4m + 3m^2)D_J + (2m + 3m^2)D_{JK} + 3m^2D_K\right]$$

$$\rho_2 = \frac{3}{32c_2^2B_0^4}\left[(128 + 64m + 48m^2 + 40m^3 + 35m^4)D_J^2 + 2(16m + 24m^2 + 30m^3 + 35m^4)D_JD_{JK} + 2(8m^2 + 20m^3 + 35m^4)\left(D_JD_K + \tfrac{1}{2}D_{JK}^2\right) + 2(10m^3 + 35m^4)D_{JK}D_K + 35m^4D_K^2\right]$$

where $m = B_0/A_0$.

**For asymmetrical top molecules, (see ref. 8)

$$\rho = -\frac{1}{16c_2}\left[3\left(\frac{\tau_{aaaa}}{A_0^2} + \frac{\tau_{bbbb}}{B_0^2} + \frac{\tau_{cccc}}{C_0^2}\right) + 2\left(\frac{\tau_{aabb}}{A_0B_0} + \frac{\tau_{bbcc}}{B_0C_0} + \frac{\tau_{aacc}}{A_0C_0}\right) + 4\left(\frac{\tau_{abab}}{A_0B_0} + \frac{\tau_{bcbc}}{B_0C_0} + \frac{\tau_{acac}}{A_0C_0}\right)\right]$$

For planar molecules $\tau_{bcbc} = \tau_{acac} = 0$, and also the following relations hold:

$$\tau_{aacc} = \left(\frac{C_0}{A_0}\right)^2\tau_{aaaa} + \left(\frac{C_0}{B_0}\right)^2\tau_{aabb}\ ; \qquad \tau_{bbcc} = \left(\frac{C_0}{B_0}\right)^2\tau_{bbbb} + \left(\frac{C_0}{A_0}\right)^2\tau_{aabb}\ ; \qquad \tau_{cccc} = \left(\frac{C_0}{A_0}\right)^2\tau_{aacc} + \left(\frac{C_0}{B_0}\right)^2\tau_{bbcc}$$

TABLE III. - TERMS IN $\ln Q_c^m$

Formula number	Method: PANDK[a] and JANAF[b]	Method: NRRAO1[c]	Method: NRRAO2[d]	$\ln Q^m$ terms[e]	Remarks: Type of molecule: Diatomic	Linear polyatomic	Nonlinear	Remarks: Definitions
8	No	Yes	Yes	$\sum_{i=1}^{n} d_i a_i r_i s_i \left[1 + \frac{1}{2} a_i s_i + \frac{1}{6} a_i^2 s_i^2 (1 + r_i)\right]$				d_i = degeneracy
								$r_i = d^{-u_i}$
								$u_i = c_2 \nu_i / T$
								$s_i = 1/(1 - r_i)$
								n = number of unique frequencies
					Yes	No	No	$\nu_1 = \omega_e - 2\omega_e x_e + 3.25\omega_e y_e + 5\omega_e z_e$
					Yes	No	No	$a_1 = (\alpha_1 - \alpha_2 - 0.75\alpha_3)/B_0$
					No	Yes	No	$a_i = \frac{\alpha_i^B}{B_0} - \sum_{j=1}^{n} \frac{(1 + \delta_{ij})\alpha_{ij}}{2B_0}$
					No	No	Yes	$a_i = \frac{1}{2}\left(\frac{\alpha_i^A}{A_0} + \frac{\alpha_i^B}{B_0} + \frac{\alpha_i^C}{C_0}\right)$
9	Yes	No	No	$\sum_{i=1}^{n} d_i P_i r_i s_i$	Yes	Yes	No	$P_i = a_i(a_i + 1)$
					Yes	No	No	For PANDK, $a_1 = (\alpha_1 - 2\alpha_2 - 3.25\alpha_3)/B_0$ and for JANAF, $a_1 = (\alpha_1 - \alpha_2 - 0.75\,\alpha_3)/B_e$
					No	No	Yes	$P_i = a_i\left(\frac{a_i}{2} + 1\right) + \frac{1}{4}\left[\left(\frac{\alpha_i^A}{A_0}\right)^2 + \left(\frac{\alpha_i^B}{B_0}\right)^2 + \left(\frac{\alpha_i^C}{C_0}\right)^2\right]$
10	No	Yes	Yes	$\sum_{i=1}^{n} \left[d_i a_{ii} r_i s_i^2 (a_i s_i + a_i r_i s_i + 1) + \sum_{j>1}^{n} d_i d_j a_{ij} r_i r_j s_i s_j + \sum_{j=1}^{n} d_i d_j a_i a_{ij} (1 + \delta_{ij}) r_i r_j s_i^2 s_j\right]$	Yes	No	No	$a_{11} = \left(-\alpha_2 - \frac{3}{2}\alpha_3\right)/B_0$
					No	Yes	No	$a_{ij} = \alpha_{ij}/B_0$
					No	No	Yes	$a_{ij} = 0$
					Yes	Yes	Yes	$\delta_{ij} = \begin{cases} 0 \text{ for } i \neq j \\ 1 \text{ for } i = j \end{cases}$

TABLE III. - Continued.

Formula number	Method			$\ln Q^m$ terms[e]	Remarks			
					Type of molecule			Definitions
	PANDK[a] and JANAF[b]	NRRAO1[c]	NRRAO2[d]		Diatomic	Linear polyatomic	Nonlinear	
11	No	Yes	Yes	$a_{111}r_1s_1^3(1 + 4r_1 + r_1^2)$ (diatomics only)	Yes	No	No	$a_{111} = -\alpha_3/B_0$
12	No	Yes	Yes	$-\frac{c_2}{T}\sum_{\substack{i=1\\j=i}}^{n} d_i(d_j + \delta_{ij})X_{ij}r_ir_js_is_j$	Yes	No	No	For PANDK, $X_{11} = -\omega_e x_e + 4.5\omega_e y_e + 14.5\omega_e z_e$ and for JANAF, $X_{11} = (-\omega_e x_e + 4.5\omega_e y_e + 14.5\omega_e z_e)\nu_1/\omega_e$
					No	Yes	Yes	$X_{ii} = x_{ii} + (1.5\,d_i + 3)y_{iii} + \sum_{\substack{k=1\\k\neq i}}^{n}\frac{d_k}{2}y_{iik}$
					No	Yes	Yes	$X_{ij} = x_{ij} + (d_i + 1)y_{iij} + (d_j + 1)y_{ijj} + \sum_{\substack{k=1\\k\neq i}}^{n}\frac{d_k}{2}y_{ijk}$
13	No	Yes	Yes	$-\frac{c_2}{T}\sum_{\substack{i=1\\j=i\\k=j}}^{n} d_i(d_j + \delta_{ij})(d_k + \delta_{ik} + \delta_{jk})Y_{ijk}r_ir_jr_ks_is_js_k$	Yes	No	No	$Y_{111} = \omega_e y_e + 8\omega_e z_e$
					No	Yes	Yes	$Y_{ijk} = y_{ijk}$
14	Yes	No	No	$-\frac{c_2}{T}\sum_{\substack{i=1\\j=i}}^{n} d_i(d_j + \delta_{ij})(X_{ij} + G_i)r_ir_js_is_j$	Yes	No	No	$G_i = 0$
					No	Yes	Yes	$G_i = \begin{cases} 0 \text{ if } i \neq j \\ (g_{ii} + B_0)/3 \text{ if } i = j \end{cases}$
15	No	Yes	Yes	$-\frac{24c_2}{T}\omega_e z_e r_1^4 s_1^4$ (diatomics only)				
16	No	Yes	Yes	$-\frac{c_2}{T}\sum_{i=1}^{n} 2g_{ii}r_is_i^2(1 - 2a_ir_is_i)$				
17	No	Yes	Yes	$-\frac{c_2}{T}\sum_{\substack{i=1\\j=1}}^{n} d_i(d_j + \delta_{ij})(1 + \delta_{ij})a_iX_{ij}r_ir_js_i^2s_j$				

TABLE III. - Continued.

Formula number	Method			$\ln Q^m$ terms[e]	Remarks			
					Type of molecule			Definitions
	PANDK[a] and JANAF[b]	NRRAO1[c]	NRRAO2[d]		Diatomic	Linear polyatomic	Nonlinear	
18	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{\substack{i=1 \\ j=i}}^{n} d_i(d_j + \delta_{ij})(1 + \delta_{ij})X_{ij}^2 r_i r_j s_i^2 s_j^2$				
19	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{\substack{i=1 \\ j=1 \\ k=j}}^{n} \mathscr{D}_{ijk} X_{ij} X_{ik} r_i r_j r_k s_i^2 s_j s_k$	Yes	Yes	Yes	$\mathscr{D}_{ijk} = (2 - \delta_{jk})(1 + \delta_{ij})(1 + \delta_{ik})d_i(d_j + \delta_{ij})(d_k + \delta_{ik})$
20	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{\substack{i=1 \\ j=i \\ k=1}}^{n} \mathscr{D}_{ijk} X_{ij} Y_{ijk} r_i r_j r_k s_i^2 s_j^2 s_k$	Yes	Yes	Yes	$\mathscr{D}_{ijk} = 2(1 + \delta_{ij})(1 + \delta_{ik} + \delta_{jk})(d_i + \delta_{ij})d_j(d_k + \delta_{ik} + \delta_{jk})$
21	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{\substack{i=1 \\ j=1 \\ k=1 \\ \ell=k}}^{n} \mathscr{D}_{ijk\ell} X_{ij} Y_{ik\ell} r_i r_j r_k r_\ell s_i^2 s_j s_k s_\ell$	Yes	Yes	Yes	$\mathscr{D}_{ijk\ell} = 2(1 + \delta_{ij})(1 + \delta_{ik} + \delta_{i\ell})d_i(d_j + \delta_{ij})(d_k + \delta_{ik}) \times (d_\ell + \delta_{i\ell} + \delta_{k\ell})$
22	No	No	Yes	$\left(\frac{c_2}{T}\right)^2 \sum_{i=1}^{n} g_{ii}^2 r_i s_i^4 (1 + 8r_i + r_i^2)$				
23	No	No	Yes	$\left(\frac{c_2}{T}\right)^2 \sum_{\substack{i=1 \\ j=1}}^{n} 2g_{ii} X_{ij} r_i r_j s_i^3 s_j [1 + 7\delta_{ij} + r_i(1 + 5\delta_{ij})]$				
24	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{i=1}^{n} 4a_i [X_{ii} d_i (d_i + 1)]^2 r_i^5 s_i^5$				
25	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{\substack{i=1 \\ j=1}}^{n} \mathscr{D}_{ij} a_i X_{ij}^2 r_i r_j s_i^3 s_j^2$	Yes	Yes	Yes	$\mathscr{D}_{ij} = (1 + \delta_{ij})^2 d_i (d_j + \delta_{ij})$

TABLE III. - Concluded.

Formula number	Method			$\ln Q^m$ terms[e]	Remarks			
	PANDK[a] and JANAF[b]	NRRAO1[c]	NRRAO2[d]		Type of molecule			Definitions
					Diatomic	Linear polyatomic	Nonlinear	
26	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} \mathscr{D}_{ijk} a_i X_{ij} X_{ik} r_i r_j r_k s_i^3 s_j s_k (1 + r_i)$	Yes	Yes	Yes	$\mathscr{D}_{ijk} = (1 + \delta_{ij})(1 + \delta_{ik}) d_i (d_j + \delta_{ij})(d_k + \delta_{ik})$
27	No	No	Yes	$\frac{1}{2}\left(\frac{c_2}{T}\right)^2 \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} \mathscr{D}_{ijk} a_i X_{ij} X_{jk} r_i r_j r_k s_i^2 s_j^2 s_k$	Yes	Yes	Yes	$\mathscr{D}_{ijk} = (1 + \delta_{ij})(1 + \delta_{jk})(2 - \delta_{ik}) d_i (d_j + \delta_{ij})[(1 + \delta_{ik}) d_k + \delta_{ik} + \delta_{jk} + \delta_{ij}\delta_{jk}]$

[a] Modified Pennington and Kobe method.
[b] Joint Army Navy Air Force method.
[c] Nonrigid-Rotator Anharmonic-Oscillator 1.
[d] Nonrigid-Rotator Anharmonic-Oscillator 2.

[e] Derivatives: $T\left[d\left(\ln Q_c^m\right)/dT\right] = \sum_j \ln Q_{c_j} S_j$ and $T^2\left[d^2\left(\ln Q_c^m\right)/dT^2\right] = \sum_j \ln Q_{c_j}\left[\sum_i m_i u_{h_i}^2 r_{h_i} s_{h_i}\left(r_{h_i} s_{h_i} + 1\right) - 2S_j + S_j^2 - p_j\right]$

where $\ln Q_c^m = \sum_j \ln Q_{c_j}$ and $\ln Q_{c_j}$ is any term in formulas 8 to 27 which has the formula $\ln Q_{c_j} = (c_2/T)^{p_j} C_j \prod_i r_{h_i}^{n_i} s_{h_i}^{m_i}$

where $p_j = 0$, 1, or 2; C_j is a constant; n_i and m_i are integer exponents; and h_i is an integer subscript, and where

$S_j = \sum_i u_{h_i}\left(n_i + m_i r_{h_i} s_{h_i}\right) - p_j$.

TABLE IV. - BRIEF DESCRIPTION OF CONTENTS OF INPUT RECORDS

Record ID	Labels	Numerical value	Comments	Optional?
CTEM			Gives temperature schedule for tables calculated from coefficients if different than original data.	Yes
	T	T, K	This may be a single value or the beginning or end of an interval.	Yes
	I	T increment, K	This must be preceded by a lower and followed by a higher T value.	
data	(See table VII)		All data records following a METHOD record must have the same record ID including the possibility of all blanks. Contents of the remainder of the record may vary with method.	No
DATE	(Any six characters)	(blank)	Label will appear in the least-squares coefficients output.	Yes
FINISH	(blank)	(blank)	Indicates the end of a set of input data for a species.	No
formula	See comments	See comments	Chemical formula of species (columns 1 to 12). For remainder of record, see table V. (The word "formula" does not appear on the record.)	No
LISTEF	(blank)	(blank)	Calls for listing contents of EF data sets stored in I/O unit 13.	Yes
LSTSQS	[a]EXP	T exponent	q_i values in eq. (11).	Yes
	[a]NOCNS	(blank)	Fit is to be made with no constraints.	Yes
	[a]NOCP	(blank)	No heat capacities to be used in least-squares fit.	Yes
	[a]NOH	(blank)	No enthalpies to be used in least-squares fit.	Yes
	[a]NOS	(blank)	No entropies to be used in least-squares fit.	Yes
	OLD	(blank)	Use "old" polynomial form for eq. (11) (e.g., q_i = 0,1,2,3,4).	Yes
	T	T, K	Temperature at the beginning or end of interval to be fit.	Yes
	TCONST	Constraint T, K	Calls for the data at this temperature to be fitted exactly. Numerical value of T must be the same as some value in the T schedule. Default value is 298.15 K.	Yes
	TPROP	Properties T, K	Used in conjunction with NOH and/or NOS. Specifies temperature at which a value of enthalpy and/or entropy is given to obtain integration constants.	Yes
METHOD	------	------	See table VI for details.	No
NAME	------	------	Columns 7-24 are reserved for species name and columns 25-80 for comments. Both to be included with coefficients. See table VIII.	Yes
OUTPUT	ATM	(blank)	Calls for pressure to be in units of atmospheres. (Default units are bars.)	Yes
	CAL	(blank)	Calls for the energy units in the tables to be calories.	Yes
	CTAB	(blank)	Calls for tables of functions calculated from coefficients.	Yes
	DMLESS	(blank)	Calls for many-figured tables in dimensionless units.	Yes
	EFTAPE	(blank)	Calls for the H_0^o value as well as the $\Delta_f H_T^o$ and $-(G_T^o - H_0^o)/RT$ data to be put on I/O units 11 and 13 for future $\log_{10} K$ and $\Delta_f H_T^o$ calculations.	Yes
	INTERM	(blank)	Calls for intermediate output data.	Yes
	JOULES	(blank)	Calls for the energy units in the tables to be joules.	Yes
	LOCK	(blank)	Calls for rounded tables including columns for $\Delta_f H_T^o$ and $\log_{10} K$.	Yes
	LSQS	(blank)	Calls for least-squared fit of functions.	Yes
	MFIG	(blank)	Calls for tables of many-figured functions.	Yes
REFNCE	Any alphanumeric characters	Any alphanumeric characters	----------	Yes
TEMP	T	Temperature, K	This may be a single value or the beginning or end of an interval.	Yes

[a]May require an integer in column 80. See discussion in section "LSTSQS record."

TABLE V. - CONTENTS OF FORMULA RECORDS

Labels 2, 3, or 4		Numerical value	Comments
HF298	Use only one	An assigned enthalpy, $H^o_{298.15}$	Numerically equal to heat of formation at 298.15 K
ASINDH		An assigned enthalpy, H^o_T	Requires corresponding temperature
DELTAH		Heat of formation from the assigned reference elements $(\Delta_f H^o_T)$	Requires corresponding temperature
T		Temperature	Not required with HF298
CAL	Use only one	(Blank)	Units are cal/mol
KCAL		(Blank)	Units are kcal/mol
JOULES		(Blank)	Units are J/mol
KJOULE		(Blank)	Units are kJ/mol
INVCM		(Blank)	Units are cm^{-1}/mol
EV		(Blank)	Units are eV/mol

TABLE VI. - CONTENTS OF METHOD RECORDS

Type of species	Method code (any label)	Labels 1,2,3, or 4	Numerical value	Comments
All	COEF		(blank)	Calculate functions from empirical equations.
		DMLESS	(blank)	Coefficients on data records are those of eqs. (11) to (13).
		MELTPT	Melting point	See MELTPT under READIN.
		DELTAH	Heat of transition	Used between two phases of the same species; code is on METHOD record of second phase.
		DELTAS	Entropy of transition	May be used in lieu of a heat of transition (see label DELTAH).
		CAL	(blank)	See READIN below.
		JOULES	(blank)	See READIN below.
		KCAL	(blank)	See READIN below.
		KJOULE	(blank)	See READIN below.
All	READIN		(blank)	Read in functions directly.
		H298HO	$H^o_{298.15} - H^o_0$	Used in obtaining $H^o_T - H^o_0$ values when $H^o_T - H^o_{298.15}$ values are given.
		MELTPT	Melting point	Optional information when a set of input data has both solid and liquid phases.
		CAL	(blank)	Energy units of properties on METHOD and following data records are calories.
		JOULES	(blank)	Energy units of properties on METHOD and following data records are joules.
		KCAL	(blank)	Energy units for enthalpies on METHOD and following data records are kilocalories. Other properties are in calories.
		KJOULE	(blank)	Energy units for enthalpies on METHOD and following data records are kilojoules. Other properties are in joules.

TABLE VI. - Concluded.

Type of species	Method code (any label)	Labels 1,2,3, or 4	Numerical value	Comments
Monatomic gases	ALLN		(blank)	Include all levels given in input.
		GLABEL	(blank)	Labels in data records are $g_m = 2]_m + 1$ (eq. (7)).
		FILL	(blank)	See FILL option under FIXEDN.
Monatomic gases	FIXEDN		Highest principal quantum number to be included in calculations	All energy levels whose principal quantum number is less than or equal to this number will be included.
		GLABEL	(blank)	See GLABEL option under ALLN.
		FILL	(blank)	Missing energy levels will be estimated and included as discussed in the section "Inclusion of predicted levels."
Monatomic gases	TEMPER		(blank)	Cut off all levels above "reduced" ionization potential. (See section "Internal Partition Function for Monatomic Gases.")
		GLABEL	(blank)	See GLABEL option under ALLN.
		FILL	(blank)	See FILL option under FIXEDN.
Diatomic and polyatomic gases	ADD	(blank)	(blank)	No labels for this method.
Diatomic and polyatomic gases	JANAF		(blank)	Calculation method of ref. 6 (see tables II and III).
Diatomic and polyatomic gases	WILH	LINE	(blank)	Wilhoit extrapolation method. LINE required only for linear molecules.
Diatomic and polyatomic gases	NRRAO1		(blank)	Calculation method of refs. 30 and 31 (see tables II and III).
Diatomic and polyatomic gases	NRRAO2		(blank)	Same as NRRAO1 with some higher order corrections (see tables II and III).
Diatomic and polyatomic gases	PANDK		(blank)	Calculation method of ref. 29 (see tables II and III).
Diatomic and polyatomic gases	RRHO		(blank)	Rigid-rotator harmonic-oscillator approximation (see table II).

TABLE VII. - CONTENTS OF DATA RECORDS

Method	Labels 1, 2, 3, or 4	Numerical value	Comments
ADD	(Group name)	Quantity of that group	The group names are given in table IX. Each group name is followed by the quantity of that group in the species.
	SYMNO	Symmetry number	Taken to be 1 if omitted.
	STATWT	Statistical weight	Taken to be 1 if omitted.
	HRCO	H_T^o/R correction	Any adjustment to H_T^o/R.
	SRCO	S_T^o/R correction	Any adjustment to S_T^o/R.
READIN	T	Temperature, K	One value on each record.
	CP	C_p^o	Either one of these values on each record.
	CP/R	C_p^o/R	
	H-H0	$H_T^o - H_0^o$	Any one of these values on each record.
	H-H2	$H_T^o - H_{298.15}^o$	
	H-H0/T	$(H_T^o - H_0^o)/T$	
	H-H2/T	$(H_T^o - H_{298.15}^o)/T$	
	H-H0RT	$(H_T^o - H_0^o)/RT$	
	H-H2RT	$(H_T^o - H_{298.15}^o)/RT$	
	S	S_T^o	Any one of these values on each record.
	S/R	S_T^o/R	
	-G-H0	$-(G_T^o - H_0^o)$	
	-G-H2	$-(G_T^o - H_{298.15}^o)$	
	-GH0/T	$-(G_T^o - H_0^o)/T$	
	-GH2/T	$-(G_T^o - H_{298.15}^o)/T$	
	-GH0RT	$-(G_T^o - H_0^o)/RT$	
	-GH2RT	$-(G_T^o - H_{298.15}^o)/RT$	
COEF	See comments	----------	First record may be the same as aforementioned READIN record with C_p^o or C_p^o/R value omitted. The data will be used in obtaining the integration constants, b_1 and b_2, in eqs. (12) and (13).
	T	Temperature at beginning or end of temperature range	Two T labels must precede exponents and coefficients for the temperature range.
	Ei(i = 1, 2,..., or 8)	q_i in eq. (11)	----------
	Ci(i = 1, 2,..., or 8)	a_i or $a_i \times R$ in eq. (11)	a_i with DMLESS code in METHOD record.
	CH	$b_1 \times R$ in eq. (12)	Use one if b_1 has not been set by previous enthalpy value.
	CH/R	b_1 (eq. (12))	
	CH-H0	$b_1 \times R - H_0^o$ (eq. (12))	
	CHH0/R	$b_1 - H_0^o/R$ (eq. (12))	
	CS	$b_2 \times R$ (eq. (13))	Use one if b_2 has not been set by previous entropy value.
	CS/R	b_2 (eq. (13))	
	TCOEF	Temperature at beginning or end of temperature range included with coefficient output	Calls for coefficients to be written on I/O units 6 and 10 in same format as least-squares coefficients. Temperature values should be omitted if they are the same as the T values above.
FIXEDN, ALLN, or TEMPER[a]	IP	Ionization potential in cm^{-1}	Required only with TEMPER.
	J_m value	ε_m/hc in cm^{-1} (eq. (7))	J_m value (1) Does not have to be right or left-adjusted. (2) May be integer, 0, or decimal number (if decimal, it can have only 5 or 0 to right of decimal point). (3) Must not be left blank (if 0, type in 0).

[a]For FILL option (METHOD record) or FIXEDN, the principal quantum number for the data on each record must be in columns 79 to 80, right-adjusted.

TABLE VII. - Continued.

Method	Labels 1, 2, 3, or 4	Numerical value	Comments
RRHO, PANDK, JANAF, NRRAO1, or NRRAO2[b]	SYMNO	Symmetry number.	Taken to be 1 if omitted.
	STATWT	Statistical weight	Taken to be 1 if omitted.
	TO	T_0, cm^{-1}	Use with excited electronic state.
	BO	B_0, cm^{-1}	B_e, B_0, or I_B value must be included for all molecules.
	BE	B_e, cm^{-1}	See comments for label BO. Use only for linear molecules.
	WE	ω_e, cm^{-1}	Diatomics only.
	WEXE	$\omega_e x_e$, cm^{-1}	
	WEYE	$\omega_e y_e$, cm^{-1}	
	WEZE	$\omega_e z_e$, cm^{-1}	
	WX4	Anharmonic constant one order higher than $\omega_e z_e$, cm^{-1}	
	ALPHAE	α_e, cm^{-1}	Diatomics only. $\alpha_e \equiv \alpha_1$
	ALPHAi, ($i \leq 3$)	α_i	$B_v = B_e - \alpha_1\left(v + \frac{1}{2}\right) + \alpha_2\left(v + \frac{1}{2}\right)^2 + \alpha_3\left(v + \frac{1}{2}\right)^3$
	ALFABi ($i \leq 6$)	α_i, cm^{-1}	Linear polyatomics only. $B_{[v]} = B_e - \sum_{i=1}^{n\leq 6}\left[\alpha_i\left(v_i + \frac{d_i}{2}\right) - \sum_{j\geq 1}^{n\leq 6}\alpha_{ij}\left(v_i + \frac{d_i}{2}\right)\left(v_j + \frac{d_j}{2}\right)\right]$
	Aij ($i,j \leq 6$)	α_{ij}, cm^{-1}	
	ALFAAi ($i \leq 6$)	α_i^A, cm^{-1}	Nonlinear molecules only. $A_{[v]} = A_e - \sum_{i=1}^{n\leq 6}\alpha_i^A\left(v_i + \frac{d_i}{2}\right)$ where v_i and d_i are the vibrational quantum number and degeneracy respectively for the i^{th} fundamental frequency.
	ALFABi ($i \leq 6$)	α_i^B, cm^{-1}	Nonlinear molecules only. $B_{[v]} = B_e - \sum_{i=1}^{n\leq 6}\alpha_i^B\left(v_i + \frac{d_i}{2}\right)$
	ALFACi ($i \leq 6$)	α_i^C, cm^{-1}	Nonlinear molecules only. $C_{[v]} = C_e - \sum_{i=1}^{n\leq 6}\alpha_i^C\left(v_i + \frac{d_i}{2}\right)$
	DE	D_e, cm^{-1}	Diatomics only.
	BETAi ($i \leq 3$)	β_i, cm^{-1}	Diatomics only, where $D_v = D_e - \beta_1\left(v + \frac{1}{2}\right) + \beta_2\left(v + \frac{1}{2}\right)^2 + \beta_3\left(v + \frac{1}{2}\right)^3$
	Vi(d_i) or Vi ($i \leq 20$)	$\nu_i(d_i)$ or ν_i, cm^{-1}	d_i is degeneracy (an integer) of ν_i and may be omitted when $d_i = 1$.
	Xij ($i \leq 6$, $j \leq 6$)	x_{ij}, cm^{-1}	Polyatomics only.
	Yijk ($i \leq 6$, $j \leq 6$, $k \leq 6$)	y_{ijk}, cm^{-1}	Polyatomics only.
	WO	W_0 (Fermi resonance constant), cm^{-1}	Linear polyatomics only.
	Gii ($i \geq 6$)	g_{ii}, cm^{-1}	Linear polyatomics only.
	DO or D000	D_0 or D_{000}	Polyatomics only.
	RHO	ρ, K^{-1}	Polyatomics only.
	AO	A_0, cm^{-1}	An I_A or A_0 must be included for all nonlinear polyatomics.
	CO	C_0, cm^{-1}	An I_C or C_0 must be included for all nonlinear polyatomics.
	IB	$I_B \times 10^{39}$, $(g)(cm^2)$	$B_0 = h/8\pi^2 cI_B = 2.7992774 \times 10^{-39}/I_B$. See comments for label BO.
	IA	$I_A \times 10^{39}$, $(g)(cm^2)$	$A_0 = h/8\pi^2 cI_A = 2.7992774 \times 10^{-39}/I_A$. See comments for label AO.
	IC	$I_C \times 10^{39}$, $(g)(cm^2)$	$C_0 = h/8\pi^2 cI_C = 2.7992774 \times 10^{-39}/I_C$. See comments for label CO.

[b]For excited electronic states, the data for each state should be put on separate records with an identifying number in columns 79 to 80. Data records for each state must be grouped together.

TABLE VII. - Concluded.

Method	Labels 1, 2, 3, or 4	Numerical value	Comments
RRHO, PANDK, JANAF, NRRAO1, or NRRAO2[b] (concluded)	IAIBIC	$I_A I_B I_C \times 10^{117}$, $(g)^3(cm)^6$	Replaces individual values for I_A, I_B, and I_C.
	INTROT	Total number of internal rotors	Remaining labels in this table, which appear on records following the INTROT record, are parameters pertaining to internal rotation. Integer in column 79 or 80 indicates to which rotor parameters belong (maximum of four unique rotors).
	ANGLES	<201	The number of phase angles in 2π radians (see eq. (10)). If number is not assigned, default value is 201.
	BROT	B_0, cm^{-1}	Same as B_0 but for internal rotation BROT = $2.7992774 \times 10^{-39}/I_B$.
	NEL	<187	Number of energy levels to be calculated. Default is 187.
	NOUT	<187	Number of energy levels to be printed. Default is 0.
	NROTOR	1, 2, 3, or 4	Integer specifying the number of rotors with identical parameters.
	ROSYM	Rotor symmetry number	
	V	Potential, cm^{-1}	See eq. (10).
	Vn ($n \leq 6$)	V_n	n-fold barrier V_n (see eq. (10)).
	IPRINT		Calls for listing the potential corresponding to the various phase angles. (Not used to obtain the partition function.)

[b]For excited electronic states, the data for each state should be put on separate records with an identifying number in columns 79 to 80. Data records for each state must be grouped together.

TABLE VIII. - GENERAL THERMODYNAMIC COEFFICIENTS FORMAT

General Format:

Record	Contents	Format	Columns
1	Species name or formula	A24	1 to 24
	Comments - data source	A56	25 to 80
2	Number of T intervals	I2	2
	Optional identification code	A6	4 to 9
	Chemical formula, symbols and numbers	5(A2,F6.2)	11 to 50
	0 for gas and non-zero for condensed	I1	52
	Molecular weight	F13.5	53 to 65
	Heat of formation at 298.15 K, J/mol	F15.3	66 to 80
3	Temperature range	2F10.3	2 to 21
	Number of coefficients for C_p^o	I1	23
	T exponents in empirical equation for C_p^o	8F5.1	24 to 63
	$H^o_{298.15} - H^o_0$, J/mol	F15.3	66 to 80
4	First five coefficients	5D16.8	1 to 80
5	Last three coefficients for C_p^o	3D16.8	1 to 48
	Integration constants for H^o_T/RT and S^o_T/R	2D16.8	49 to 80
...	Repeat 3, 4, and 5 for each interval.		

Example:

```
SIH+              SILYLIDYNE ION.  JANAF DEC, 1971.
 2 J12/71 SI  1.00H   1.00E  -1.00    0.00    0.00 0      29.09289    1147671.200
    298.150  1000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8654.259
-4.28447370d+04  3.85838948d+02  2.55865994d+00 -6.98804091d-04  5.22573029d-06
-4.84510719d-09  1.45288897d-12  0.00000000d+00  1.34921190d+05  8.95659370d+00
  1000.000  6000.000 7 -2.0 -1.0  0.0  1.0  2.0  3.0  4.0  0.0          8654.259
 1.70438606d+05 -1.04392569d+03  4.83677344d+00  1.28725833d-04 -6.90835693d-08
 1.42207295d-11 -7.87210915d-16  0.00000000d+00  1.43159900d+05 -7.53965976d+00
```

Empirical equations for above example (from eqs. (11) to (13)):

$$\text{Heat capacity:} \quad \frac{C_p^o}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4$$

$$\text{Enthalpy:} \quad \frac{H_T^o}{RT} = -a_1 T^{-2} + a_2 T^{-1} \ln T + a_3 + a_4 \frac{T}{2} + a_5 \frac{T^2}{3} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{b_1}{T}$$

$$\text{Entropy:} \quad \frac{S_T^o}{R} = -a_1 \frac{T^{-2}}{2} - a_2 T^{-1} + a_3 \ln T + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + b_2$$

TABLE IX. - GROUP NOTATION AND STRUCTURE

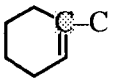
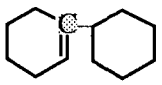
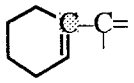
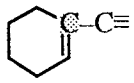
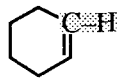
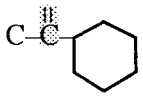
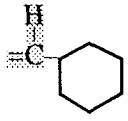
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
1	CA	C_a		C	36
2	CBC	$C_B - (C)$		C	36
3	CBCB	$C_B - (C_B)$		C	37
4	CBCD	$C_B - (C_d)$		C	37
5	CBCT	$C_B - (C_t)$		C	37
6	CBH	$C_B - (H)$		CH	37
7	CDC2	$C_d - (C)_2$		C	36
8	CDCBC	$C_d - (C_B)(C)$		C	36
9	CDCDC	$C_d - (C_d)(C)$		C	36
10	CDHC	$C_d - (H)(C)$		CH	36
11	CDHCB	$C_d - (C_B)(H)$		CH	37

TABLE IX. - Continued.

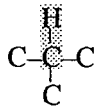
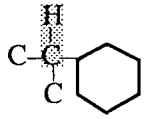
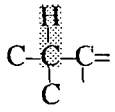
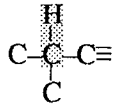
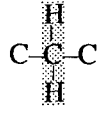
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
12	CDHCD	$C_d - (C_d)(H)$		CH	37
13	CDHCT	$C_d - (C_t)(H)$		CH	37
14	CDH2	$C_d - (H)_2$		CH_2	37
15	CHC3	$C - (H)(C)_3$		CH	36
16	CHCBC2	$C - (C_B)(C)_2(H)$		CH	36
17	CHCDC2	$C - (C_d)(C)_2(H)$		CH	36
18	CHCTC2	$C - (C_t)(C)_2(H)$		CH	36
19	CH2C2	$C - (H)_2(C)_2$		CH_2	36

TABLE IX. - Continued.

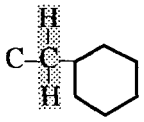
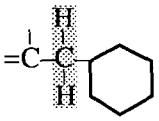
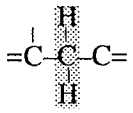
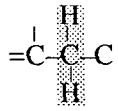
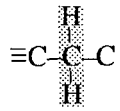
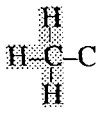
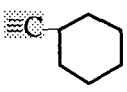
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
20	CH2CBC	C - $(C_B)(C)(H)_2$		CH_2	36
21	CH2CBD	C - $(C_d)(C_B)(H)_2$		CH_2	36
22	CH2CD2	C - $(C_d)_2(H)_2$		CH_2	36
23	CH2CDC	C - $(C_d)(C)(H)_2$		CH_2	36
24	CH2CTC	C - $(C_t)(C)(H)_2$		CH_2	36
25	CH3C	C - $(H)_3(C)$		CH_3	36
26	CTC	C_t - (C)		C	36
27	CTCB	C_t - (C_B)		C	37

TABLE IX. - Concluded.

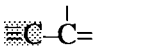
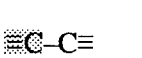
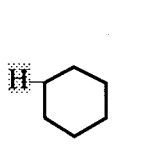
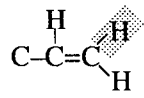
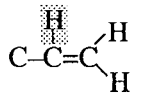
Group number	PAC91 group label	Benson notation (ref. 36)	Structure	Atoms contained in group	Reference for thermodynamic data
28	CTCD	$C_t - (C_d)$		C	37
29	CTCT	$C_t - (C_t)$		C	37
30	CTH	$C_t - (H)$		CH	37
31	HC2H	H - ACETYL		H	see "Input"
32	HPHEN	H - PHENYL		H	see "Input"
33	HVIN	H - VINYL		H	see "Input"
34	HVINS	H - STABILIZED VINYL		H	see "Input"

TABLE X. - GROUP ADDITIVITY COEFFICIENTS

```
CA
 2 BEN76  C   1.00    0.00    0.00    0.00    0.00 0     12.01100      17210.010
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  6.20131064d-01  6.55685438d-03 -8.40971939d-06  5.34237173d-09 -1.34221334d-12
                                                  1.67980617d+04 -2.13964424d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  1.70014134d+00  2.13036557d-03 -1.46491180d-06  4.57867726d-10 -5.30959813d-14
                                                  1.65796625d+04 -7.34011722d+00
CBC
 2 BEN76  C   1.00    0.00    0.00    0.00    0.00 0     12.01100       2772.724
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  1.10379898d+00 -1.40207754d-03  1.01721889d-05 -1.04915786d-08  3.35530569d-12
                                                  2.43522265d+03 -1.01067689d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  1.18859776d+00  2.62679100d-03 -1.40397450d-06  3.62315999d-10 -3.62315999d-14
                                                  2.15954456d+03 -1.17034055d+01
CBCB
 2 S&F85  C   1.00H   0.00    0.00    0.00    0.00 0     12.01100          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 -9.07225320d-01  1.21274570d-02 -1.59921140d-05  1.06772290d-08 -2.88771260d-12
                                                  2.34891290d+03 -2.17231890d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  1.64937250d+00  2.43505820d-03 -1.40110120d-06  3.74624350d-10 -3.82283850d-14
                                                  1.78059830d+03 -1.47139470d+01
CBCD
 2 S&F85  C   1.00H   0.00    0.00    0.00    0.00 0     12.01100          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  1.89361290d+00 -3.63320180d-03  1.33476670d-05 -1.32062840d-08  4.38875210d-12
                                                  2.36121080d+03 -1.41160640d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  6.57951850d-01  3.79153180d-03 -2.18052300d-06  5.80353650d-10 -5.87829120d-14
                                                  2.50341600d+03 -8.72472110d+00
CBCT
 2 S&F85  C   1.00H   0.00    0.00    0.00    0.00 0     12.01100          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  1.89361290d+00 -3.63320180d-03  1.33476670d-05 -1.32062840d-08  4.38875210d-12
                                                  2.36121080d+03 -1.58018030d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  6.57951850d-01  3.79153180d-03 -2.18052300d-06  5.80353650d-10 -5.87829120d-14
                                                  2.50341600d+03 -1.04104590d+01
CBH
 2 S&F85  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 -8.59079180d-01  1.01575080d-02 -6.05790130d-06  1.11817290d-10  8.76799660d-13
                                                  1.51812920d+03  7.93471810d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  8.12920500d-01  5.70326930d-03 -2.94688640d-06  7.32625720d-10 -7.11722860d-14
                                                  1.07063610d+03 -6.86258470d-01
CDC2
 2 BEN76  C   1.00    0.00    0.00    0.00    0.00 0     12.01100       5203.260
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  1.57567141d-02  1.20990725d-02 -2.39398157d-05  2.39017773d-08 -9.01711547d-12
                                                  4.82932602d+03 -9.21726687d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  2.25642353d+00  1.36203978d-03 -7.27986777d-07  1.87867555d-10 -1.87867555d-14
                                                  4.34871092d+03 -1.99090723d+01
```

TABLE X. - Continued.

```
CDCBC
 2 BEN76  C   1.00    0.00    0.00    0.00    0.00 0     12.01100       4347.792
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.15050677d+00  2.56218701d-02 -4.82075840d-05  4.17875044d-08 -1.37198166d-11
                                                 4.19996194d+03 -9.32804085d-01
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 3.04446083d+00  4.86442777d-04 -2.59995277d-07  6.70955554d-11 -6.70955554d-15
                                                 3.27765919d+03 -2.51782099d+01
CDCDC
 2 BEN76  C   1.00    0.00    0.00    0.00    0.00 0     12.01100       4468.564
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.15050677d+00  2.56218701d-02 -4.82075840d-05  4.17875044d-08 -1.37198166d-11
                                                 4.32073394d+03 -9.32804085d-01
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 3.04446083d+00  4.86442777d-04 -2.59995277d-07  6.70955554d-11 -6.70955554d-15
                                                 3.39843119d+03 -2.51782099d+01
CDHC
 2 BEN76  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894       4322.631
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 3.87658435d-01  6.91462635d-03 -4.92473068d-06  3.06564147d-09 -1.19103098d-12
                                                 3.93773106d+03 -6.55229555d-02
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 1.76953318d+00  3.63735034d-03 -1.32392850d-06  1.71399542d-10 -2.18997389d-15
                                                 3.48001920d+03 -7.46676354d+00
CDHCB
 2 S&F85  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-1.77479380d+00  2.03672900d-02 -2.92063140d-05  2.13900470d-08 -6.19476560d-12
                                                 3.25431500d+03  8.37139370d+00
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 2.16078460d+00  3.89973620d-03 -1.87505280d-06  4.40575310d-10 -4.10819930d-14
                                                 2.44872450d+03 -1.05679580d+01
CDHCD
 2 S&F85  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-1.77479380d+00  2.03672900d-02 -2.92063140d-05  2.13900470d-08 -6.19476560d-12
                                                 3.25431500d+03  8.37139370d+00
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 2.16078460d+00  3.89973620d-03 -1.87505280d-06  4.40575310d-10 -4.10819930d-14
                                                 2.44872440d+03 -1.05679580d+01
CDHCT
 2 S&F85  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-1.77479380d+00  2.03672900d-02 -2.92063140d-05  2.13900470d-08 -6.19476560d-12
                                                 3.25431500d+03  9.20168260d+00
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 2.16078460d+00  3.89973620d-03 -1.87505280d-06  4.40575310d-10 -4.10819930d-14
                                                 2.44872450d+03 -9.73766950d+00
CDH2
 2 S&F85  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 7.08636360d-01  5.71738370d-03  3.97432860d-06 -8.14882140d-09  3.39759220d-12
                                                 2.66405290d+03  8.03997270d+00
  1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 7.62035270d-01  7.90072810d-03 -3.83366760d-06  9.04921890d-10 -8.42780610d-14
                                                 2.55458540d+03  7.24431290d+00
```

TABLE X. - Continued.

```
CHC3
 2 BEN76  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894       -956.112
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-1.21199942d+00  1.57135839d-02 -1.58129928d-05  8.16308832d-09 -1.79427286d-12
                                                -1.16875169d+03 -3.21908314d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 4.21180248d+00  8.18242540d-05  1.33950798d-06 -6.69862359d-10  9.41347774d-14
                                                -2.66361789d+03 -3.11576551d+01
CHCBC2
 2 BEN76  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894       -493.152
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.70626696d+00  2.55442809d-02 -3.35585641d-05  2.09055818d-08 -5.02705367d-12
                                                -5.64094599d+02  3.00591586d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 3.92458678d+00  2.09170394d-03 -1.11797969d-06  2.88510888d-10 -2.88510888d-14
                                                -2.12756082d+03 -2.99433080d+01
CHCDC2
 2 BEN76  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894       -744.761
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.69178809d+00  2.27174202d-02 -2.67597650d-05  1.50516772d-08 -3.18914467d-12
                                                -7.43740880d+02  3.74363064d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 2.00129268d+00  5.30222627d-03 -2.83394852d-06  7.31341554d-10 -7.31341554d-14
                                                -1.74761503d+03 -1.92282945d+01
CHCTC2
 2 BEN76  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894       -865.533
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.29967144d+00  2.07315703d-02 -2.60278088d-05  1.75696487d-08 -4.99182528d-12
                                                -9.03749304d+02  2.30198068d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
1  1.48247630d+00  5.93460188d-03 -3.17194238d-06  8.18565776d-10 -8.18565777d-14
                                                -1.70025797d+03 -1.60989330d+01
CH2C2
 2 BEN76  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688       -2480.858
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 2.95576901d-01  8.26548665d-03  2.02730929d-06 -8.22251499d-09  3.84394234d-12
                                                -2.93983603d+03  5.66809199d-01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 8.95359335d-01  8.82630650d-03 -4.51610338d-06  1.11218836d-09 -1.07950628d-13
                                                -3.18218807d+03 -2.98904913d+00
CH2CBC
 2 BEN76  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688       -2445.633
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-1.61079486d+00  2.13020824d-02 -2.44229173d-05  1.42423100d-08 -3.20026830d-12
                                                -2.72304502d+03  8.49250374d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 2.81096829d+00  5.93460188d-03 -3.17194238d-06  8.18565777d-10 -8.18565777d-14
                                                -3.81247249d+03 -1.36149824d+01
CH2CBD
 2 BEN76  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688       -2158.799
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.99489148d+00  2.49586869d-02 -2.77613624d-05  1.47398773d-08 -2.60172081d-12
                                                -2.15783856d+03  1.58638825d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 1.17752700d+00  8.75596999d-03 -4.67991499d-06  1.20772000d-09 -1.20772000d-13
                                                -3.03586486d+03 -4.40568818d+00
```

TABLE X. - Continued.

```
CH2CD2
 2 BEN76  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688      -2158.799
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-2.99489148d+00  2.49586869d-02 -2.77613624d-05  1.47398773d-08 -2.60172081d-12
                                                -2.15783856d+03  1.58638825d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 1.17752700d+00  8.75596999d-03 -4.67991499d-06  1.20772000d-09 -1.20772000d-13
                                                -3.03586486d+03 -4.40568818d+00
CH2CDC
 2 BEN76  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688      -2395.311
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-9.84166104d-01  1.41467063d-02 -7.15413971d-06 -2.15080256d-09  2.42261065d-12
                                                -2.66434595d+03  6.65325780d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 8.87674198d-01  9.14512421d-03 -4.88791121d-06  1.26139644d-09 -1.26139644d-13
                                                -3.13410437d+03 -2.90870113d+00
CH2CTC
 2 BEN76  C   1.00H   2.00    0.00    0.00    0.00 0     14.02688      -2380.215
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-7.61851269d-01  1.30343429d-02 -7.51763250d-06  4.44629802d-10  9.34733367d-13
                                                -2.66730666d+03  5.96602298d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 3.68857816d-01  9.77749982d-03 -5.22590507d-06  1.34862066d-09 -1.34862066d-13
                                                -2.94558197d+03  2.32409280d-01
CH3C
 2 BEN76  C   1.00H   3.00    0.00    0.00    0.00 0     15.03482      -5132.810
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 9.67091211d-01  4.54272496d-03  1.40931220d-05 -2.03529587d-08  8.18255263d-12
                                                -5.71121159d+03  7.97556073d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
-6.27511183d-01  1.36690420d-02 -7.30586729d-06  1.88538511d-09 -1.88538511d-13
                                                -5.43213903d+03  1.52438529d+01
CTC
 2 BEN76  C   1.00    0.00    0.00    0.00    0.00 0     12.01100      13863.619
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 8.02437417d-01  3.49837285d-03 -4.15397270d-06  4.07988802d-09 -1.75083632d-12
                                                 1.34983448d+04 -2.26753348d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 1.24244195d+00  2.09170394d-03 -1.11797969d-06  2.88510888d-10 -2.88510888d-14
                                                 1.33531243d+04 -4.58500863d+00
CTCB
 2 S&F85  C   1.00H   0.00    0.00    0.00    0.00 0     12.01100          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
-3.49384520d+00  2.72321320d-02 -4.76891040d-05  3.86559630d-08 -1.19225380d-11
                                                 1.33155360d+04  1.68245410d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 2.28560130d+00  8.22574900d-04 -4.14361390d-07  1.03588260d-10 -1.03983680d-14
                                                 1.22382860d+04 -1.04535180d+01
CTCD
 2 S&F85  C   1.00H   0.00    0.00    0.00    0.00 0     12.01100          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
 7.72587840d-01  1.44159610d-03  2.24535910d-06 -3.27337130d-09  1.18176800d-12
                                                 1.38820450d+04 -1.66930970d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
 4.49136330d-01  3.36057940d-03 -1.88820530d-06  4.95862840d-10 -4.98295890d-14
                                                 1.39278700d+04 -2.35699140d-01
```

TABLE X. - Concluded.

```
CTCT
 2 S&F85  C   1.00H   0.00    0.00    0.00    0.00 0     12.01100          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  9.09050340d-03  9.68282400d-03 -1.61930660d-05  1.34477210d-08 -4.31250880d-12
                                                  1.25675030d+04  6.29563560d-01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  1.61375010d+00  1.75286410d-03 -9.50741270d-07  2.44108940d-10 -2.42282270d-14
                                                  1.22902950d+04 -6.81710090d+00
CTH
 2 S&F85  C   1.00H   1.00    0.00    0.00    0.00 0     13.01894          0.000
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0
  3.22062990d-01  1.23444940d-02 -1.94881630d-05  1.58382730d-08 -4.95581450d-12
                                                  1.30498420d+04  7.64972930d+00
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0
  2.08408360d+00  3.00946820d-03 -1.27530500d-06  2.64569910d-10 -2.18420530d-14
                                                  1.27910130d+04 -3.35539540d-01
HVIN              C2H4 - C2H3
 2 L 2/91 H   1.00    0.00    0.00    0.00    0.00 0     1.00794    -625071.953
    200.000  1000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
  7.46735360d-01 -9.08531026d-03  3.11780593d-05 -3.33930685d-08  1.22733472d-11
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -7.52125326d+04 -2.33376993d+00
   1000.000  6000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
 -3.59257940d-01  2.99014152d-03 -1.07409461d-06  1.73348003d-10 -1.03738147d-14
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -7.53284072d+04  1.23891111d+00
HVINS             C2H4 - C2H3 + 8 kcal correction on H.
 2 L 2/91 H   1.00    0.00    0.00    0.00    0.00 0     1.00794    -591599.953
    200.000  1000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
  7.46735360d-01 -9.08531026d-03  3.11780593d-05 -3.33930685d-08  1.22733472d-11
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -7.11867993d+04 -2.33376993d+00
   1000.000  6000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
 -3.59257940d-01  2.99014152d-03 -1.07409461d-06  1.73348003d-10 -1.03738147d-14
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -7.13026738d+04  1.23891111d+00
HPHEN             C6H6 - C6H5
 2 L 1/91 H   1.00    0.00    0.00    0.00    0.00 0     1.00794    -254320.000
    200.000  1000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
 -2.06302352d-01 -8.15243200d-04  1.43769315d-05 -1.95955059d-08  8.17474280d-12
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -3.05819013d+04  1.10333770d+00
   1000.000  6000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
  3.06920100d-01  2.32195120d-03 -8.16396860d-07  1.29838420d-10 -7.68981960d-15
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -3.08941277d+04 -2.51191430d+00
HC2H              C2H2 - C2H1
 2 L 3/91 H   1.00    0.00    0.00    0.00    0.00 0     1.00794    -331613.472
    298.150  1000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
 -3.22796852d+00  1.87214852d-02 -3.02272137d-05  2.39352994d-08 -7.26880375d-12
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -3.95302119d+04  1.38493147d+01
   1000.000  3000.000 5  0.0  1.0  2.0  3.0  4.0  0.0  0.0  0.0           0.000
 -5.51834000d-02  3.11952519d-03 -1.41953706d-06  3.15909714d-10 -2.79158072d-14
  0.00000000d+00  0.00000000d+00  0.00000000d+00 -4.00479060d+04 -8.06478801d-01
```

TABLE XI. - INDEX OF INPUT RECORD ID'S AND LABELS

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
ADD	Label	2	VI	6,10,17,18,19,23,24
ALLN	Label		VI,VII	6,10,15,16,19,22
ALPHAE	Label		VII	
ALPHAi	Label	7	VII	
ALFABi	Label		VII	
ALFAij	Label		VII	
ALFAAi	Label	5	VII	
ALFABi	Label	5	VII	
ALFACi	Label	5	VII	
ANGLES[a]	Label		VII	
ASINDH[a]	Label	5	V	18
ATM	Label	3	IV	11,19
AO	Label	5	VII	
BAR	Label	3		11
BE	Label	7	VII	
BETAi	Label		VII	
BROT	Label		VII	
BO	Label	5	VII	
Ci	Label	6,8	VII	
CAL	Label	1,4,5,8	IV,V,VI	9,19,21
CH	Label		VII	
CH/R	Label		VII	
CH-HO	Label		VII	
CHHO/R	Label		VII	
COEF	Label	6,8	VI,VII	10,11,16,19,24
CP	Label	3,6,8	VII	
CP/R	Label		VII	
CS	Label		VII	
CS/R	Label		VII	
CTAB	Label	1,6,7	IV	9,19,21
CTEM	Record ID	6,7	IV	8,9,12,15,16,21,24
CO	Label	5	VII	

[a]Program checks first four characters only.

TABLE XI. - Continued.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
data	Any record ID	1-8	IV,VI,VII	9,10,11,15,16,17,18,19,21
DATE	Record ID	1-4,6-8	IV	9,15,17,24
DE	Label		VII	
DELTAH	Label	6,8	V,VI	7,12,16
DELTAS	Label		VI	7,12,16
DMLESS[a]	Label	1,3,4	IV,VI	9,19,21
DO	Label		VII	
DOOO	Label		VII	
Ei	Label	6,8	VII	
EFDA	Record ID			8,10,11,15,17,23
EFTAPE[a]	Label	6	IV	9,10,17,19,21,23
EV	Label		V	
EXP	Label	1,2	IV	7,10,18
FILL	Label	1	I,VI,VII	6,12,16,22
FINISH[a]	Record ID	1-8	IV	8,9,10,15,17,24
FIXEDN[a]	Label		VI,VII	6,10,15,16,19,22
formula[b]	Variable record ID and label	1-8	IV,V	9,15,17,24
-G-HO	Label		VII	
-GHO/T	Label		VII	
-GHORT	Label		VII	
-G-H2	Label		VII	
-GH2/T	Label		VII	
-GH2RT	Label		VII	
Gii	Label		VII	
GLABEL[a]	Label		VI	16
H-HO	Label	3,6	VII	
H-HO/T	Label		VII	
H-HORT	Label		VII	
H-H2	Label	6,8	VII	
H-H2/T	Label		VII	

[a]Program checks first four characters only.
[b]First 12 columns of record are reserved for chemical formula.

TABLE XI. - Continued.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
H-H2RT	Label		VII	
H298HO	Label	2,6,8	VI	16
HF298	Label	1,3,4,6,7,8	V	10,18
HRCO	Label		VII	11,17
I	Label	1,2,4-8	IV	16,20
IA	Label		VII	
IAIBIC[a]	Label	4	VII	
IB	Label	4	VII	
IC	Label		VII	
INTERM[a]	Label	5	IV	10,11,19,22
INVCM[a]	Label		V	
INTROT[a]	Label	4	VII	11
IP	Label	1	VII	
IPRINT[a]	Label		VII	
J_m[c]	Numerical label	1	VII	10
JANAF[a]	Label	7	II,III,VI,VII	6,11,16,17,19,22,24
JOULES[a]	Label	1-8	IV,V,VI	9,19,21
KCAL	Label	8	V,VI	
KJOULE[a]	Label	3	V,VI	
LINE	Label		VI	7,19,33
LISTEF[a]	Record ID		IV	8,10,16,18,21,23
LOGK	Label	7,8	IV	9,11,17,18,19,21,23
LSQS	Label	1,2,6,7,8	IV	9,10,11,18,19,21,23
LSTSQS[a]	Record ID	1,2	IV	6,7,8,9,15,16,18,19,40,45
MELTPT[a]	Label	6,8	VI	
METHOD[a]	Record ID	1-8	IV,VI	6,7,8,9,10,11,12,15,16,18, 19,20,22,23,24
MFIG	Label	1-6	IV	9,12,19,21
NAME	Record ID	1-4,6-8	IV	8,9,11,15,19,24,30
NEL	Label	4	VII	
NOCNS[a]	Label		IV	7,18

[a]Program checks first four characters only.
[c]Labels are numerical values of J_m or g_m (eq. (7)).

TABLE XI. - Continued.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
NOCP	Label		IV	16,18,19
NOH	Label		IV	16,18,19
NOS	Label		IV	16,18,19
NOUT	Label		VII	11
NROTOR[a]	Label	4	VII	
NRRAO1	Label		II,III,VI,VII	6,11,16,19,22,38
NRRAO2	Label	5	II,III,VI,VII	6,11,16,17,19,22,24
OLD	Label		IV	18
OUTPUT[a]	Record ID	1-8	IV	8,9,10,11,12,15,17,18,19, 21,22,23,24
PANDK[a]	Label		II,III,VI,VII	6,8,11,16,19,22
READIN[a]	Label	3,6,8	VI	9,11,16,19,20,24
REFNCE[a]	Record ID	1,3-6	IV	8,9,15,20,24
RHO	Label	5	VII	
ROSYM[a]	Label	4	VII	
RRHO	Label	4	II,VI,VII	6,11,15,16,17,19,22,24
S	Label	3,6,8	VII	
S/R	Label		VII	
SRCO	Label		VII	
STATWT[a]	Label	2,4,5,7	VII	15
SYMNO[a]	Label	2,5	VII	
T	Label	1-8	IV,V,VII	10,16,18,19,20
TCOEF[a]	Label	6,8	VII	10,16
TCONST[a]	Label		IV	18
TEMP	Record ID	1-6,8	IV	8,9,12,15,16,19,20,24,45
TEMPER[a]	Label	1	VI,VII	6,10,15,16,19,24
TPROP[a]	Label		IV	18
TO	Label	7	VII	
V	Label		VII	
Vi	Label	4,5	VII	
VN	Label		VII	
WE	Label	7	VII	
WEXE	Label	7	VII	

[a]Program checks first four characters only.

TABLE XI. - Concluded.

Input code	Type	Example number (appendix D)	Table number	Pages where discussed
WEYE	Label		VII	
WEZE	Label		VII	
WX4	Label		VII	
WILH	Label	2,3	VI	7,12,16,19,24
WO	Label		VII	
Xij	Label	5	VII	
Yijk	Label	5	VII	

a_1	a_2	a_3	a_4	a_5	a_6	a_7	$b_1 - \frac{H_0^\circ}{R}$	b_2	λ_0	λ_1	λ_2	Constants
$\frac{9}{4}\sum T^{-4}$	$\sum\left(\frac{3}{2} - \ln T\right)T^{-3}$	$-\frac{1}{2}\sum T^{-2} \ln T$	0	$\frac{5}{12}$ p	$\frac{7}{12}\sum T$	$\frac{27}{40}\sum T^2$	$-\sum T^{-3}$	$-\frac{1}{2}\sum T^{-2}$	T_0^{-2}	$-T_0^{-2}$	$-\frac{T_0^{-2}}{2}$	$\sum T^{-2}\left(\frac{C_p^\circ}{R} - \frac{H_T^\circ - H_0^\circ}{RT} - \frac{1}{2}\frac{S_T^\circ}{R}\right)$
$\sum\left(\frac{3}{2} - \ln T\right)T^{-3}$	$\sum\left[2 + (\ln T)^2\right]T^{-2}$	$\sum T^{-1}$	$\frac{1}{2}\sum \ln T$	$\sum\left(\frac{1}{2} + \frac{1}{3}\ln T\right)T$	$\sum\left(\frac{2}{3} + \frac{1}{4}\ln T\right)T^2$	$\sum\left(\frac{3}{4} + \frac{1}{5}\ln T\right)T^3$	$\sum T^{-2} \ln T$	$-\sum T^{-1}$	T_0^{-1}	$T_0^{-1}\ln T_0$	$-T_0^{-1}$	$\sum T^{-1}\left(\frac{C_p^\circ}{R} + \frac{H_T^\circ - H_0^\circ}{RT} \ln T - \frac{S_T^\circ}{R}\right)$
$-\frac{1}{2}\sum T^{-2}\ln T$	$\sum T^{-1}$	$\sum\left[2 + (\ln T)^2\right]$	$\sum\left(\frac{3}{2} + \ln T\right)T$	$\sum\left(\frac{4}{3} + \frac{1}{2}\ln T\right)T^2$	$\sum\left(\frac{5}{4} + \frac{1}{3}\ln T\right)T^3$	$\sum\left(\frac{6}{5} + \frac{1}{4}\ln T\right)T^4$	$\sum\frac{1}{T}$	$\sum \ln T$	1	1	$\ln T_0$	$\sum\left(\frac{C_p^\circ}{R} + \frac{H_T^\circ - H_0^\circ}{RT} + \frac{S_T^\circ}{R}\ln T\right)$
0	$\frac{1}{2}\sum \ln T$	$\sum\left(\frac{3}{2} + \ln T\right)T$	$\frac{9}{4}\sum T^2$	$\frac{5}{3}\sum T^3$	$\frac{35}{24}\sum T^4$	$\frac{27}{20}\sum T^5$	$\frac{p}{2}$	$\sum T$	T_0	$\frac{T_0}{2}$	T_0	$\sum T\left(\frac{C_p^\circ}{R} + \frac{1}{2}\frac{H_T^\circ - H_0^\circ}{RT} + \frac{S_T^\circ}{R}\right)$
$\frac{5}{12}$ p	$\sum\left(\frac{1}{2} + \frac{1}{3}\ln T\right)T$	$\sum\left(\frac{4}{3} + \frac{1}{2}\ln T\right)T^2$	$\frac{5}{3}\sum T^3$	$\frac{49}{36}\sum T^4$	$\frac{5}{4}\sum T^5$	$\frac{143}{120}\sum T^6$	$\frac{1}{3}\sum T$	$\frac{1}{2}\sum T^2$	T_0^2	$\frac{T_0^2}{3}$	$\frac{T_0^2}{2}$	$\sum T^2\left(\frac{C_p^\circ}{R} + \frac{1}{3}\frac{H_T^\circ - H_0^\circ}{RT} + \frac{1}{2}\frac{S_T^\circ}{R}\right)$
$\frac{7}{12}\sum T$	$\sum\left(\frac{2}{3} + \frac{1}{4}\ln T\right)T^2$	$\sum\left(\frac{5}{4} + \frac{1}{3}\ln T\right)T^3$	$\frac{35}{24}\sum T^4$	$\frac{5}{4}\sum T^5$	$\frac{169}{144}\sum T^6$	$\frac{17}{15}\sum T^7$	$\frac{1}{4}\sum T^2$	$\frac{1}{3}\sum T^3$	T_0^3	$\frac{T_0^3}{4}$	$\frac{T_0^3}{3}$	$\sum T^3\left(\frac{C_p^\circ}{R} + \frac{1}{4}\frac{H_T^\circ - H_0^\circ}{RT} + \frac{1}{3}\frac{S_T^\circ}{R}\right)$
$\frac{27}{40}\sum T^2$	$\sum\left(\frac{3}{4} + \frac{1}{5}\ln T\right)T^3$	$\sum\left(\frac{6}{5} + \frac{1}{4}\ln T\right)T^4$	$\frac{27}{20}\sum T^5$	$\frac{143}{120}\sum T^6$	$\frac{17}{15}\sum T^7$	$\frac{441}{400}\sum T^8$	$\frac{1}{5}\sum T^3$	$\frac{1}{4}\sum T^4$	T_0^4	$\frac{T_0^4}{5}$	$\frac{T_0^4}{4}$	$\sum T^4\left(\frac{C_p^\circ}{R} + \frac{1}{5}\frac{H_T^\circ - H_0^\circ}{RT} + \frac{1}{4}\frac{S_T^\circ}{R}\right)$
$-\sum T^{-3}$	$\sum T^{-2}\ln T$	$\sum\frac{1}{T}$	$\frac{p}{2}$	$\frac{1}{3}\sum T$	$\frac{1}{4}\sum T^2$	$\frac{1}{5}\sum T^3$	$\sum\frac{1}{T^2}$	0	0	$\frac{1}{T_0}$	0	$\sum\frac{1}{T}\left(\frac{H_T^\circ - H_0^\circ}{RT}\right)$
$-\frac{1}{2}\sum T^{-2}$	$-\sum T^{-1}$	$\sum \ln T$	$\sum T$	$\frac{1}{2}\sum T^2$	$\frac{1}{3}\sum T^3$	$\frac{1}{4}\sum T^4$	0	p	0	0	1	$\sum\frac{S_T^\circ}{R}$
T_0^{-2}	T_0^{-1}	1	T_0	T_0^2	T_0^3	T_0^4	0	0	0	0	0	$\left.\frac{C_p^\circ}{R}\right\|_{T=T_0}$
$-T_0^{-2}$	$T_0^{-1}\ln T_0$	1	$\frac{T_0}{2}$	$\frac{T_0^2}{3}$	$\frac{T_0^3}{4}$	$\frac{T_0^4}{5}$	$\frac{1}{T_0}$	0	0	0	0	$\left.\frac{H_T^\circ - H_0^\circ}{RT}\right\|_{T=T_0}$
$-\frac{T_0^{-2}}{2}$	$-T_0^{-1}$	$\ln T_0$	T_0	$\frac{T_0^2}{2}$	$\frac{T_0^3}{3}$	$\frac{T_0^4}{4}$	0	1	0	0	0	$\left.\frac{S_T^\circ}{R}\right\|_{T=T_0}$

Figure 1. - Simultaneous least-squares fitting of heat capacity, enthalpy, and entropy.

Heat capacity: $$\frac{C_p^\circ}{R} = a_1T^{-2} + a_2T^{-1} + a_3 + a_4T + a_5T^2 + a_6T^3 + a_7T^4.$$

Enthalpy $$\frac{H_T^\circ}{RT} = -a_1T^{-2} + a_2T^{-1}\ln T + a_3 + a_4\frac{T}{2} + a_5\frac{T^2}{3} + a_6\frac{T^3}{4} + a_7\frac{T^4}{5} + \frac{b_1}{T}.$$

Entropy: $$\frac{S_T^\circ}{R} = -a_1\frac{T^{-2}}{2} - a_2T^{-1} + a_3\ln T + a_4T + a_5\frac{T^2}{2} + a_6\frac{T^3}{3} + a_7\frac{T^4}{4} + b_2.$$

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

A computer program is described which (1) calculates thermodynamic functions (heat capacity, enthalpy, entropy, and free energy) for several optional forms of the partition function, (2) fits these functions to empirical equations by means of a least-squares fit, and (3) calculates, as a function of temperature, heats of formation and equilibrium constants. The program provides several methods for calculating ideal gas properties. For monatomic gases, three methods are given which differ in the technique used for truncating the partition function. For diatomic and polyatomic molecules, five methods are given which differ in the corrections to the rigid-rotator harmonic-oscillator approximation. A method for estimating thermodynamic functions for some species is also given.

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