Reacting Fluids Laboratory
Department of Chemical Engineering
Louisiana State University
Baton Rouge, Louisiana

A Technical Report

on

THERMODYNAMIC PROPERTIES IN POLYNOMIAL FORM FOR CARBON, HYDROGEN, NITROGEN, AND OXYGEN SYSTEMS FROM 300 TO 15000°K

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D. D. Esch, Research Associate
A. Siripong, Research Assistant
R. W. Pike, Associate Professor
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NASA-RFL-TR-70-3

Prepared under Grant NGR19-001-059

for

Langley Research Center

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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ABSTRACT

Thermodynamic properties of carbon, hydrogen, nitrogen and oxygen compounds as well as selected inerts (Neon, Argon and Helium) are fitted to general polynomial forms over the following temperature ranges: 300 to 1000°K, 1000 to 6000°K, and 6000 to 15000°K. A reference state of 298.16°K and 1.0 atmosphere was chosen with H_2, N_2, O_2, Ne, Ar, He, C (solid) and e^- as reference elements. Seven coefficients are tabulated for each of the 99 species considered and for each temperature range of interest.

ACKNOWLEDGMENTS

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NOMENCLATURE

C_p°	heat capacity per mole at constant pressure
F_T°	standard free energy of a pure substance at temperature T
H_T°	standard enthalpy of a pure substance at temperature T
H_0°	standard enthalpy of a pure substance at a temperature of 0°K
R	universal gas constant, 1.987 cal/mole°K
S_T°	standard entropy of a pure substance at temperature T
T	absolute temperature
Y_i	mole fraction of species i
$(\Delta H_f^\circ)_T$	standard heat of formation at temperature T

Subscipts:

i	refers to species
T	absolute temperature (°K)
P	constant pressure

Superscripts:

°	denotes the standard state (pure substance at 1 atmosphere pressure)

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I. INTRODUCTION

In recent years it has become increasingly important to accurately determine the equilibrium compositions of multicomponent systems at very high temperatures. In the flow-field adjacent to ablative thermal protection systems, temperatures as high as 30,000°K are not uncommon. The most widely used method for calculating equilibrium compositions for such problems is that of free energy minimization.

In order to make use of this method, the free energy of each of the components is required as a function of temperature. It is convenient, for the computer implementation of free energy minimization techniques, to have this information as polynomial curve-fits. For temperatures below 6000°K, Mcbride et.al. (Ref. 9) contains such information for many species of interest. These thermodynamic properties are based on a reference state at 298.16°K. There are also numerous reports (Refs. 8 and 12) on high temperature flow field studies in which the free energy of the species of interest for the particular study have been fitted to polynomials, frequently at a reference state of 0°K.

Two alternatives are available for the procurement of data necessary equilibrium calculations: (1) the investigator is required to search through various reports for the necessary polynomial constants, then transform these values to a consistent reference state or (2) compute the polynomial fits the free energy functions as found in a number of reports, (Refs. 2-6, 11 and 13). Both procedures involve an additional evaluation of the heats of formation for the species of interest.

It is the purpose of this report to consolidate into one source, a standard set of polynomial curve-fits of thermodynamic data for species of particular interest in high temperature studies of ablative thermal

protection systems. In the section to follow, there will be a review of the relationships between the thermodynamic properties and a discussion of the techniques used to obtain the polynomial constants as reported in Appendix A.

II. MATHEMATICAL DEVELOPMENT

In this section we will first derive from fundamental relations a convenient polynomial form for the expression of standard free energy and demonstrate several important relations which permit the evaluation of other thermodynamic properties from the same set of constants. The remainder of the section will contain a discussion of the procedure used in this work to evaluate the polynomial constants.

Evaluation of Polynomial Forms

Thermodynamic data is widely available (Refs. 2-6, 11, 13) for many substances relative to their values at absolute zero. Generally this data appears in the form of the thermodynamic functions, $(H_T^\circ - H_0^\circ)/RT$ and $(F_T^\circ - H_0^\circ)/RT$ where the superscript (°) denotes the quantity at standard state (the pure component at 1 atmosphere pressure). The properties H_T° and F_T° computed from these functions will hereafter be referred to as "standard" properties. In the discussion to follow we will first derive the required polynomial form for curve-fits of this data and then demonstrate the relationship necessary for obtaining the thermodynamic properties relative to the desired reference state of the elements at 298.16°K and one atmosphere.

Using the following thermodynamic relations at constant pressure:

$$dH^\circ = C_p^\circ dT \tag{1}$$

$$dS^\circ = \frac{C_p^\circ dT}{T} \tag{2}$$

Standard heat capacity data can be conveniently fitted to the following polynomial form:

$$C_p^\circ = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \tag{3}$$

Substituting this relation into Equation (1) and integrating gives:

$$S_T^\circ = a_1 \ln T + a_2T + \frac{a_3T^2}{2} + \frac{a_4T^3}{3} + \frac{a_5T^4}{4} + a_7 \tag{4}$$

where a_7 is an integration constant. The use of the indefinite integral here is necessary since the polynomial formulation yields an indeterminant expression at absolute zero; however, this does not present any difficulties at temperatures other than absolute zero.

The derivative of the standard free energy of a substance can be defined in terms of standard enthalpy and entropy as

$$dF^\circ = dH^\circ - d(TS^\circ) = dH^\circ - TdS^\circ - S_r dT \tag{5}$$

From Equations (1) and (2) it is noted that

$$dH^\circ = TdS^\circ \tag{6}$$

therefore

$$dF^\circ = -S_T^\circ \, dT \tag{7}$$

Integrating this expression in temperature from absolute zero with S_T° defined by Equation (4) yields the following

$$F_T^\circ - F_0^\circ = \left[a_1(\ln T - 1)T + \frac{a_2T^2}{2} + \frac{a_3T^3}{6} + \frac{a_4T^4}{12} + \frac{a_5T^5}{20} + a_7T\right] \tag{8}$$

In general, standard free energy data is tabulated in non-dimensional form. Performing this nondimensionalization by dividing by RT and noting that $F_0^\circ = H_0^\circ$ gives

$$\frac{F_T^\circ - H_0^\circ}{RT} = A_1(1 - \ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 - A_7 \tag{9}$$

where $A_1 = a_1/R$, $A_2 = a_2/R$, ..., $A_5 = a_5/R$ and $A_7 = a_7/R$.
From Equations (1) and (3) the comparable polynomial expression for standard enthalpy can be derived.

$$\frac{H_T^\circ - H_0^\circ}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 \tag{10}$$

We have thus derived polynomial expressions for the thermodynamic functions of standard entropy, enthalpy and free energy relative to 0°K. In order to determine relative values of enthalpy and free energy from these functions it is necessary to specify a reference state. It is convenient to select the elements at 298°K and one atmosphere pressure for the reference state, since this condition is most widely used. The choice of reference state is related to the determination of the thermodynamic property through the enthalpy at absolute zero, H_0°. For an element, H_0° is equivalent to the change in enthalpy from the reference temperature to absolute zero. For a compound, the heat of formation from elements must be included. Since the latter quantity is identically zero for elements we can write a general expression for H_0°.

$$H_0^\circ = (\Delta H_f)_{T_{ref}} - (H_T^\circ - H_0^\circ)_{T_{ref}} \tag{11}$$

where $(H_T^\circ - H_0^\circ)_{T_{ref}}$ is available from the tabular data to be fitted.
In non-dimensional form, this equation becomes

$$\frac{H_0^\circ}{RT} = \frac{(\Delta H_f)_{T_{ref}} - (H_T^\circ - H_0^\circ)_{T_{ref}}}{RT} \qquad (12)$$

Having defined a reference state it is a simple matter to determine the thermodynamic properties from the thermodynamic functions as follows:

$$\frac{F_T^\circ}{RT} = A_1(1 - \ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7 \qquad (13)$$

$$\frac{H_T^\circ}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T} \qquad (14)$$

where $A_6 = H_0^\circ/R = \left[(\Delta H_f)_{T_{ref}} - (H_T^\circ - H_0^\circ)_{T_{ref}}\right] / R \qquad (15)$

A summary of the polynomial expressions discussed in this section is given in Table 1. For the remainder of this section we will discuss the method used to obtain the appropriate coefficients for these polynomials.

Determination of Polynomial Coefficients

There are several procedures for obtaining the polynomial constants as required for the equations given in Table 1. McBride et.al.(Ref. 9), used a least squares technique which was simultaneously applied to all four of the thermodynamic functions. For the purpose of this report, the emphasis was placed upon the free energy fit rather than the properties in general. In the following paragraphs the procedure for determining these constants is explained.

From tabulated enthalpy functions as given in several reports, for example Refs. 2-9, the following polynomial was curve fit using a simple least squares analysis,

TABLE 1

A Summary of Related Polynomial Equations for Standard Thermodynamic Properties

Specific Heat

$$\frac{C_p^\circ}{R} = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4 \qquad (A)$$

Enthalpy

$$\frac{H_T^\circ}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T} \qquad (B)$$

Entropy

$$\frac{S_T^\circ}{R} = A_1 \ln T + A_2T + \frac{A_3}{2}T^2 + \frac{A_4}{3}T^3 + \frac{A_5}{4} + A_7 \qquad (C)$$

Free Energy

$$\frac{F_T^\circ}{RT} = A_1(1-\ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7 \qquad (D)$$

$$\frac{H_T^\circ - H_0^\circ}{RT} = B_1 + B_2T + B_3T^2 + B_4T^3 + B_5T^4 \qquad (16)$$

From Equation (10) the constants A_1 through A_5 were determined as shown below:

$$A_1 = B_1$$

$$A_2 = 2B_2$$

$$A_3 = 3B_3$$

$$A_4 = 4B_4$$

$$A_5 = 5B_5$$

The constant, A_6, was computed separately from Equation (15), the appropriate values of the heat of formation 298.16 and the relative enthalpy at the reference temperature. In Appendix B the method used for calculating the heats of formation at the reference temperature is presented. Also contained in this appendix is a tabulation of the heats of formation at 298.16°K and at 0°K for each compound considered in this report.

The value of A_7 was determined as the constant difference between the tabulated free energy data and the remaining terms of the free energy polynomial as computed from the previously determined constants.

$$A_7 = A_1(1-\ln T) - \frac{A_2}{2} - \frac{A_3T^2}{6} - \frac{A_4T^4}{12} - \frac{A_5T^5}{20} - \left(\frac{F_T^\circ - H_0^\circ}{RT}\right) \qquad (17)$$

In this report constants were evaluated at two temperature ranges for all species of interest and are listed in Appendix A. The ranges considered considered were 1000-7000°K and 5000-18000°K. The overlapping and extension of temperature ranges was necessary to overcome accuracy limitations at the extremes of the fit. For completeness, polynomial coefficients as determined by other investigators have been included for several additional species for the ranges of 300-1000°K and 1000-6000°K.

III. DISCUSSION OF RESULTS

The above procedure for determining the polynomial coefficients was implemented using a Fortran IV Computer program, a listing of which is given in Appendix C. The polynomial constants as determined by this program are given in Appendix A. As previously noted, constants from various other sources are given for additional species of interest. In Appendix D tabulations of free energy, enthalpy, heat capacity and entropy as predicted by the polynomial curvefits of this report are given for each of the species considered.

The constants which were evaluated by the method of this report give predictions of free energy and enthalpy which are accurate to a minimum of four significant figures. For most species reported, predictions are accurate to five significant figures. A random sampling of accuracy with respect to predictions of entropy and heat capacity revealed a maximum deviation of 1.58% with a mean error of 2.12%.

To further test the applicability of these results, the thermodynamic constants as determined in this study were used in several free energy minimization calculations to determine the equilibrium compositions of air and of phenolic resin-nylon composites. A comparison of these results for air at 0.68 atm. is given in Fig. 1. The thermodynamic data required for ablation products was used to compute equilibrium compositions for phenolic nylon with an elemental distribution, in mass percent, of 73.03%C, 7.29% H, 4.96% N, and 14.72% O. These results which are given in Figs. 2, 3, and 4 are in agreement with those of Stroud and Brinkley, Ref. 12. In another comparison, the equilibrium compositions of air at 1 atmosphere were then used in conjunction with predicted values of heat capacity and

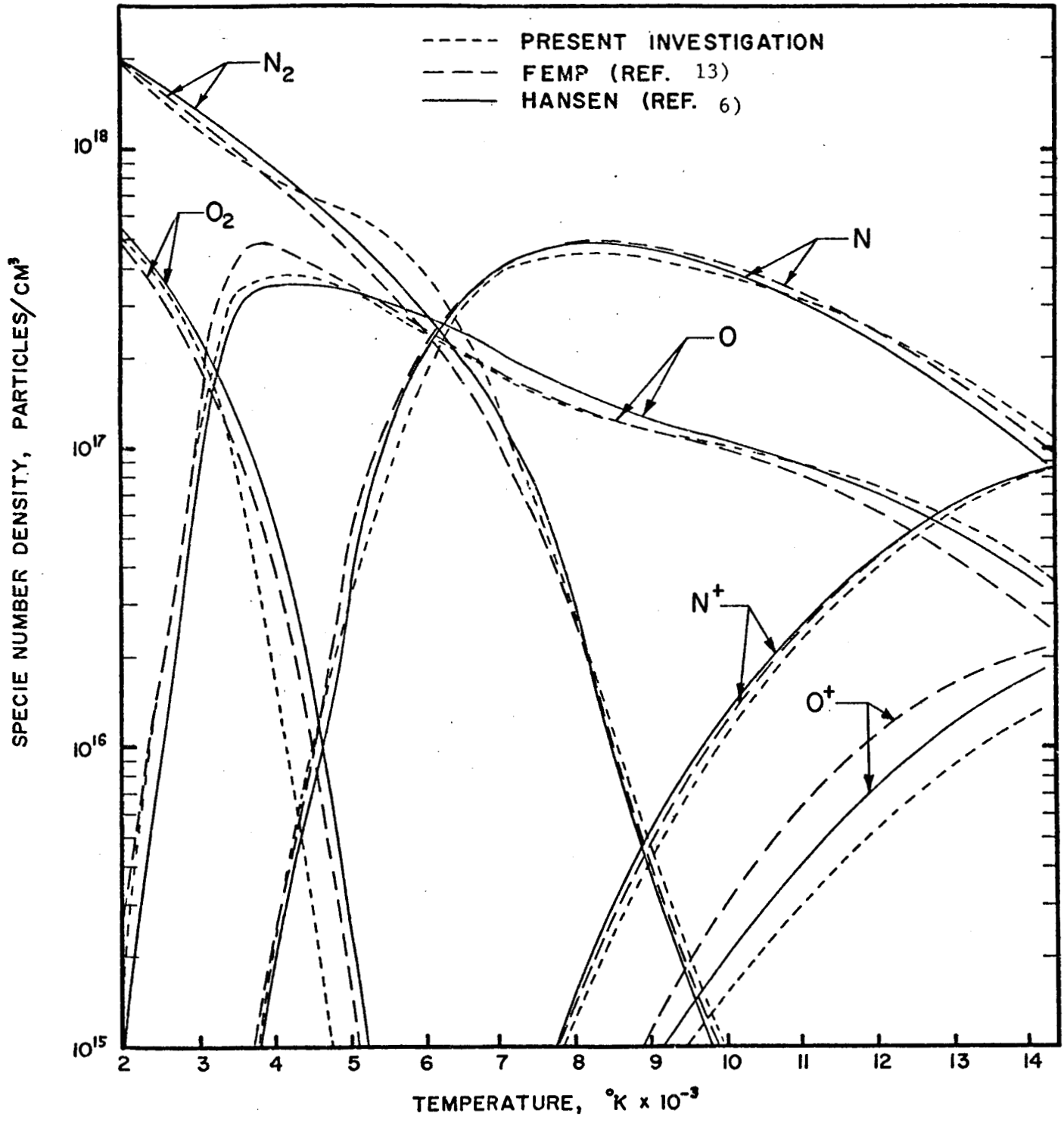

Fig. 1 Comparison of Specie Number Density Versus Temperature Calculated Using the Methods for a Pressure of .68 Atm.

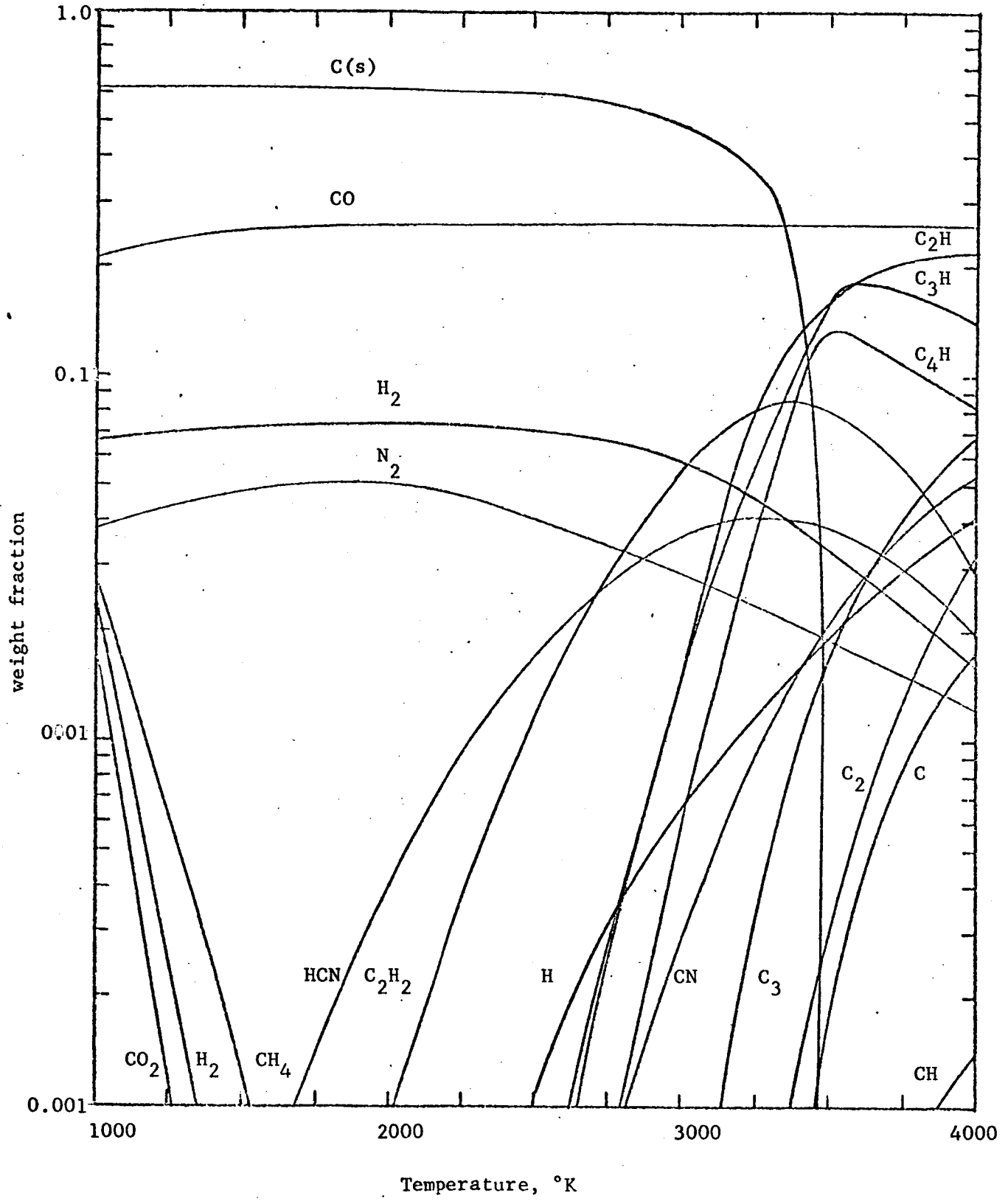

Fig. 2 Equilibrium Composition of Pyrolysis Products of Phenolic Resin-Nylon Composite at 1.0 Atmospheric Pressure

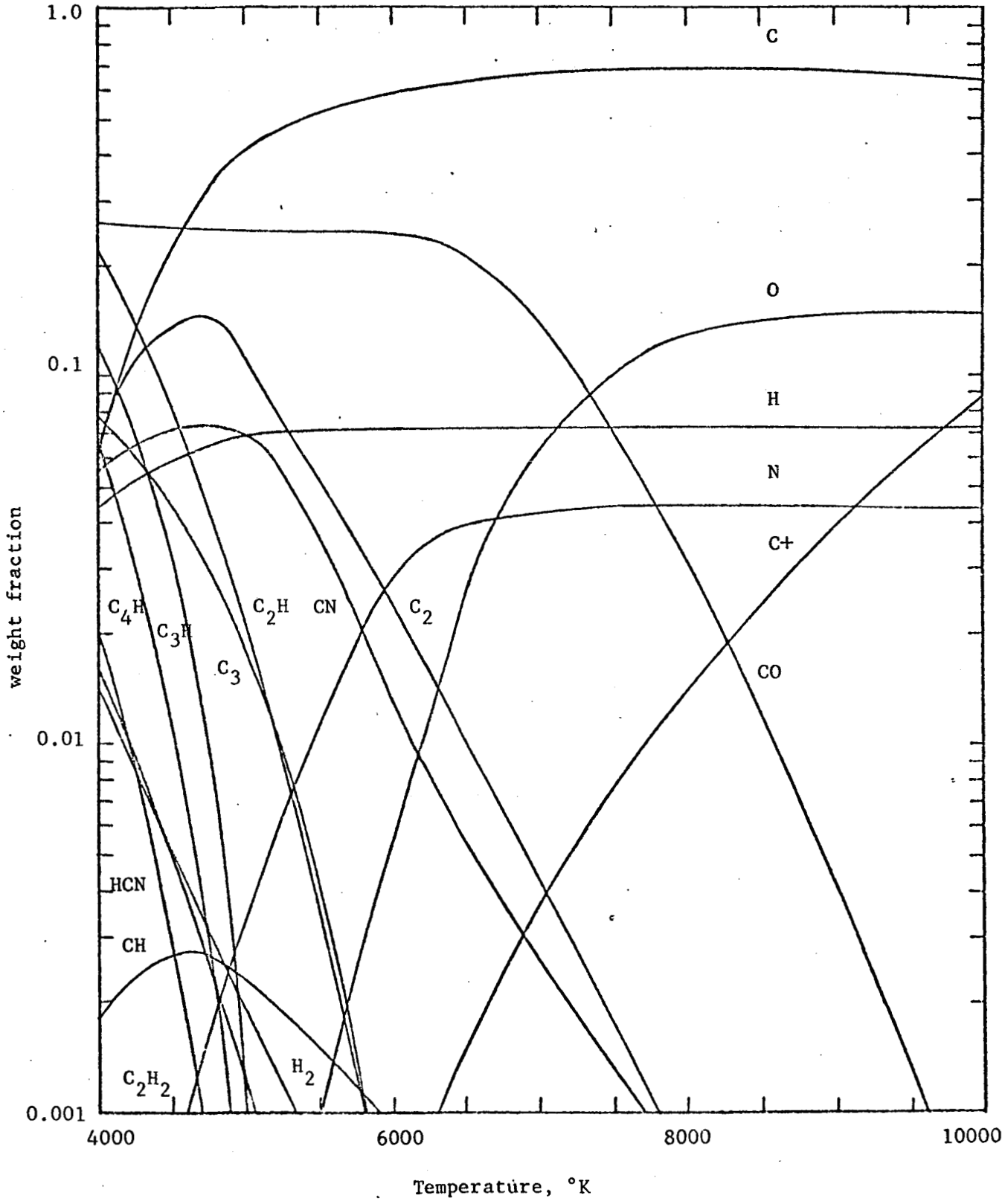

Fig. 3 Equilibrium Composition of Pyrolysis Products of Phenolic Resin-Nylon Composite at 1.0 Atmospheric Pressure

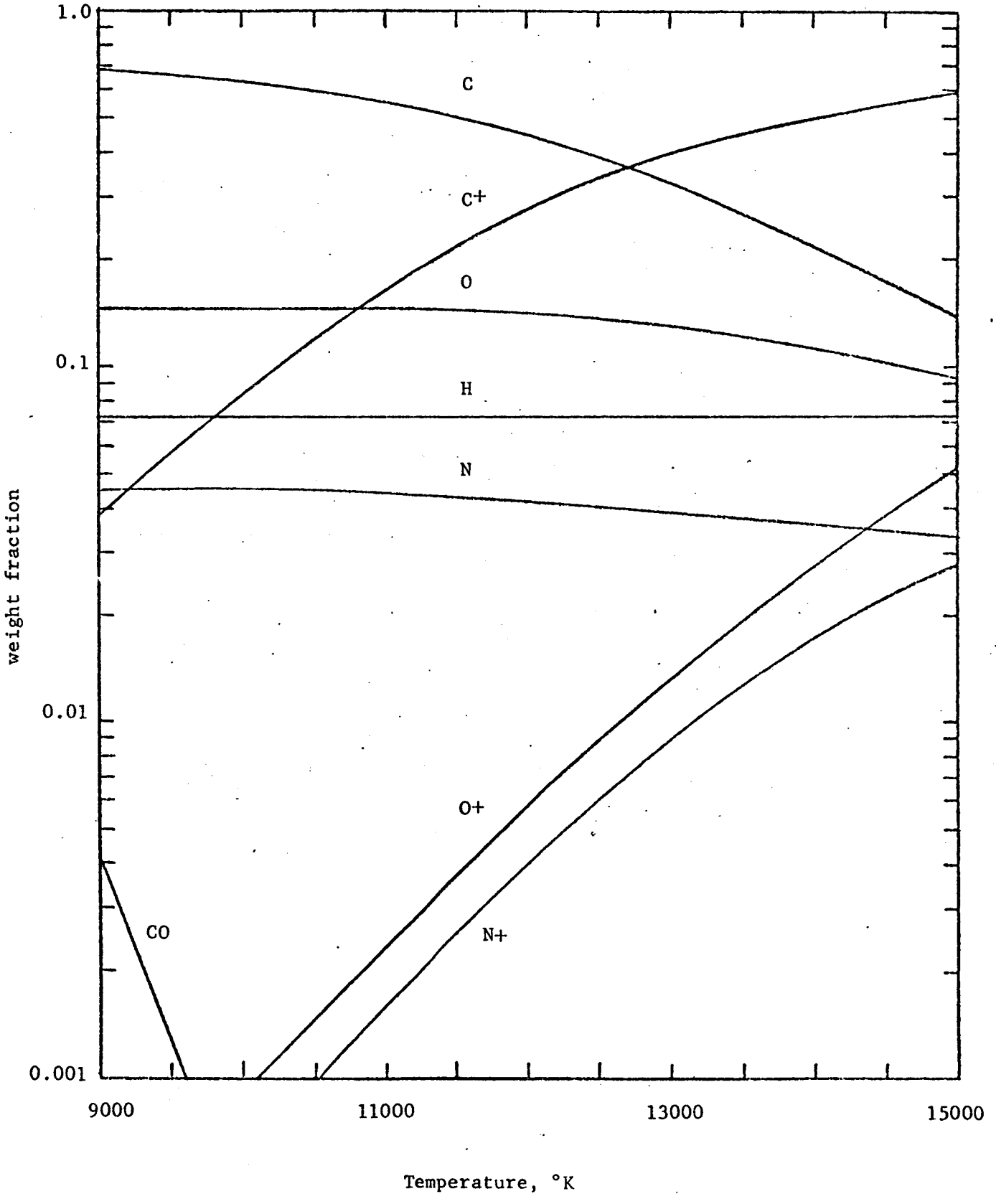

Fig. 4 Equilibrium Composition of Pyrolysis Products of Phenolic Resin-Nylon Composite at 1.0 Atmospheric Pressure

enthalpy to compute the mixture heat capacity of air by the following equation,

$$C_p^\circ = \Sigma Y_i C_{pi} + \Sigma H_i^\circ \left(\frac{\partial Y_i}{\partial T}\right) \qquad (18)$$

The results were then compared with those of other investigators as shown in Figure 5. The comparison is again quite favorable.

IV. SUMMARY

The objective of this report was to construct a standard set of polynomial curve-fits of thermodynamic data for species of interest in high temperature studies of ablating thermal protection systems. In line with this objective, polynomial coefficients for temperatures from 1000-6000°K and from 6000-15000°K were determined for 53 chemical species using the method described in Section II.

Making use of compatible curve-fits from other sources, this list was extended to 99 species, many having constants reported for three temperature ranges from 300-15000°K. Constants for the remaining species are reported either for the 300-1000°K and 1000-6000°K ranges or the 1000-6000°K and 6000-15000°K ranges. It should be noted that those species whose coefficients are not reported for a particular temperature range, are not likely to exist in equilibrium within the omitted range.

Using the computer program given in Appendix C, similar curve-fits can be obtained for any given component from tabulations of its free energy and enthalpy functions and the heat of formation of the desired component. Thus as a result of this report, a standard set of polynomial curve-fits is now available for all species of interest for studies of ablating thermal protection systems.

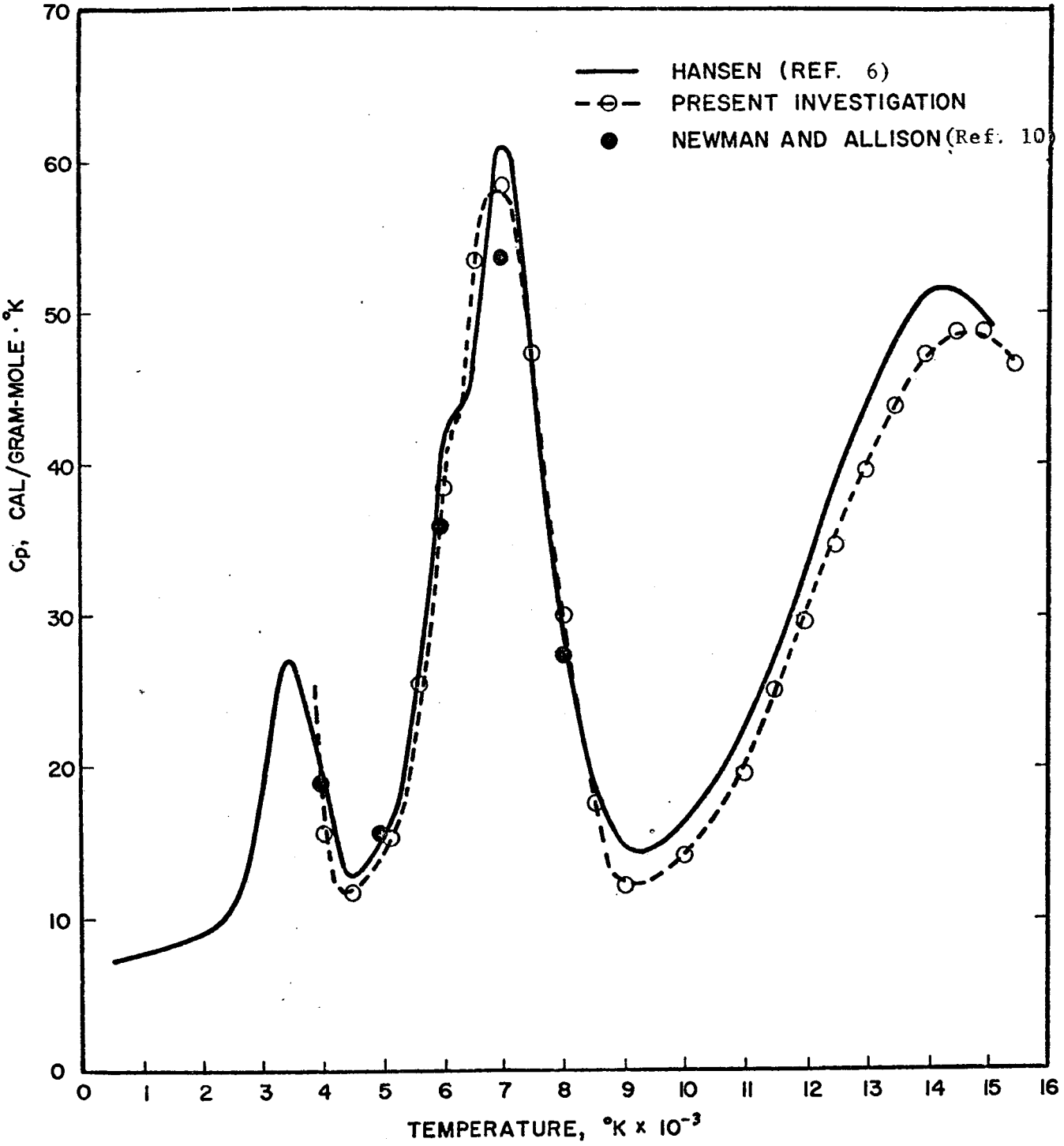

Fig. 5 Comparison of Mixture Reacting Heat Capacity for Air at 1 Atm.

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APPENDIX A

TABULATED CONSTANTS FOR POLYNOMIAL APPROXIMATIONS OF THERMODYNAMIC PROPERTIES

This appendix contains in tabular form the necessary constants for prediction of enthalpy, free energy, heat capacity and entropy, by the following equations.

$$\frac{H_T^\circ}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{6}$$

$$\frac{F_T^\circ}{RT} = A_1 (1-\ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7$$

$$\frac{C_p^\circ}{R} = A_1 + A_2T + A_3T^2 + A_4T^3 + A_5T^4$$

$$\frac{S_T^\circ}{R} = A_1 \ln T + A_2T + \frac{A_3}{2}T^2 + \frac{A_4}{3}T^3 + \frac{A_5}{4} + A_7$$

The constants, A_1 through A_7, are given in Table A-1 where the following notation is used:

SPECIE	pure component
CØDE	the reference source of data
B1, B2, B3	data source from Browne (2,3,4,5) for temperature regions 300°K to 1000°K, 1000°K to 6000°K and 6000°K to 15000°K respectively.
D1, D2	data source from Duff (4A), for temperature regions 300°K to 1000°K and 6000°K to 15000°K respectively
M1, M2	data source from McBride (9), for temperature regions 300°K to 1000°K and 1000°K to 6000°K respectively
*	constants computed in the reference shown
A1-A7	the constants for the thermodynamic functions

NOT REPRODUCIBLE

A+	0.2529E 01	0.3151E-03	-0.1961E-06	0.3988E-10	-0.2618E-14	0.1828E 06	0.5481E 01	B2
	0.2741E 01	-0.9153E-04	0.1409E-07	-0.9643E-12	0.2416E-16	0.1828E 06	0.4416E 01	B3
A++	0.2702E 01	0.1121E-03	-0.1210E-06	0.3426E-10	-0.2591E-14	0.5041E 06	0.4881E 01	B2
	0.2423E 01	0.1366E-03	-0.2538E-08	-0.8412E-12	0.3540E-16	0.5041E 06	0.6704E 01	B3
A+++	0.2478E 01	0.7329E-04	-0.5893E-07	0.1551E-10	-0.9554E-15	0.9795E 06	0.5855E 01	B2
	0.2866E 01	-0.4335E-03	0.1226E-06	-0.9547E-11	0.2329E-15	0.9795E 06	0.3669E 01	B3
A	0.2500E 01	0.1016E-05	-0.6260E-09	0.1346E-12	-0.9238E-17	-0.7454E 03	0.4367E 01	B2
	0.3078E 01	-0.5709E-03	0.1538E-06	-0.1596E-10	0.5712E-15	-0.7454E 03	0.9579E 00	B3
C+	0.2609E 01	-0.1393E-03	0.5959E-07	-0.1037E-10	0.6345E-15	0.2168E 06	0.3709E 01	B2
	0.2528E 01	0.4869E-05	-0.7026E-08	0.1134E-11	-0.3476E-16	0.2168E 06	0.4139E 01	B3
C++	0.2501E 01	-0.4142E-05	0.3365E-08	-0.9705E-12	0.9097E-16	0.5004E 06	0.2558E 01	B2
	0.2304E 01	0.2051E-03	-0.5698E-07	0.5657E-11	-0.1540E-15	0.5004E 06	0.3709E 01	B3
C+++	0.2500E 01	-0.1301E-06	0.1384E-09	-0.4498E-13	0.4405E-17	0.1057E 07	0.3257E 01	B2
	0.2469E 01	0.2978E-04	-0.7221E-08	0.5910E-12	-0.1099E-16	0.1057E 07	0.3444E 01	B3
C(S)	-0.7124E 00	0.7341E-02	-0.5526E-05	0.1514E-08	-0.2382E-13	-0.6805E 02	0.0	*M1
	0.7969E-02	0.4489E-02	-0.2569E-05	0.6697E-09	-0.6466E-13	-0.1264E 03	-0.5150E 00	*M2
C	0.2541E 01	-0.2210E-03	0.4736E-06	-0.4529E-09	0.1602E-12	0.8545E 05	0.4573E 01	*M1
	0.2612E 01	-0.2030E-03	0.1095E-06	-0.1695E-10	0.8590E-15	0.8542E 05	0.4144E 01	B2
	0.2141E 01	0.3219E-03	-0.5498E-07	0.3604E-11	-0.5564E-16	0.8542E 05	0.6874E 01	B3
C-	0.2500E 01	0.3440E-06	-0.1954E-09	0.3937E-13	-0.2573E-17	0.7083E 05	0.4356E 01	B2
	0.2508E 01	-0.6332E-05	0.1364E-08	-0.1094E-12	0.2934E-17	0.7083E 05	0.4309E 01	B3

CH	0.3545E 01	0.8795E-04	-0.1826E-05	0.4455E-08	-0.2186E-11	0.7060E 05	0.1824E 01	*M1
	0.3186E 01	0.9461E-03	-0.2442E-06	0.3107E-10	-0.1353E-14	0.7061E 05	0.3504E 01	B2
	0.3900E 01	0.1127E-03	0.2193E-07	-0.1693E-11	0.2844E-16	0.7061E 05	-0.6141E 00	B3
CH2	0.3551E 01	-0.2507E-02	0.1235E-04	-0.1175E-07	0.3812E-11	0.3366E 05	0.1797E 01	*M1
	0.3274E 01	0.2638E-02	-0.7538E-06	0.9695E-10	-0.4625E-14	0.3365E 05	0.3183E 01	B2
	0.4556E 01	0.9757E-03	-0.1478E-06	0.9828E-11	-0.2402E-15	0.3365E 05	-0.4053E 01	B3
CH3	0.3400E 01	0.4268E-02	0.2033E-06	-0.1155E-08	0.4129E-12	0.1565E 05	0.2704E 01	*M1
	0.3529E 01	0.5212E-02	-0.1680E-05	0.2399E-09	-0.1251E-13	0.1472E 05	0.1893E 01	B2
	0.6151E 01	0.1553E-02	-0.2364E-06	0.1576E-10	-0.3859E-15	0.1472E 05	-0.1272E 02	B3
CH4	0.4250E 01	-0.6913E-02	0.3160E-04	-0.2971E-07	0.9510E-11	-0.1019E 05	-0.9175E 00	*M1
	0.2234E 01	0.8929E-02	-0.2940E-05	0.4264E-09	-0.2248E-13	-0.1021E 05	0.6764E 01	B2
	0.6610E 01	0.2665E-02	-0.4192E-06	0.2880E-10	-0.7251E-15	-0.1021E 05	-0.1751E 02	B3
CN	0.3853E 01	-0.2763E-02	0.6857E-05	-0.5413E-08	0.1491E-11	0.4741E 05	0.2972E 01	*M1
	0.3411E 01	0.4897E-03	0.1005E-06	-0.3473E-10	0.2361E-14	0.4745E 05	0.4746E 01	B2
	0.3473E 01	0.7337E-03	-0.9088E-07	0.4847E-11	-0.1018E-15	0.5420E 05	0.4152E 01	B3
CO+	0.3148E 01	0.1265E-02	-0.4715E-06	0.7965E-10	-0.4421E-14	0.1490E 06	0.6051E 01	B2
	0.4076E 01	-0.1496E-03	0.1044E-06	-0.9201E-11	0.2310E-15	0.1490E 06	0.9992E 00	B3
CO	0.3787E 01	-0.2171E-02	0.5076E-05	-0.3474E-08	0.7722E-12	-0.1436E 05	0.2634E 01	*M1
	0.3254E 01	0.9098E-03	-0.2647E-06	0.3037E-10	-0.1177E-14	-0.1434E 05	0.4875E 01	B2
	0.3366E 01	0.8027E-03	-0.1968E-06	0.1940E-10	-0.5549E-15	-0.1434E 05	0.4263E 01	B3
CO2	0.2170E 01	0.1038E-01	-0.1073E-04	0.6346E-08	-0.1620E-11	-0.4835E 05	0.1066E 02	*M1
	0.4413E 01	0.3192E-02	-0.1298E-05	0.2415E-09	-0.1674E-13	-0.4894E 05	-0.7288E 00	*M2

COS	0.2089E 01	0.1461E-01	-0.2046E-04	0.1506E-07	-0.4446E-11	-0.1762E 05	0.1237E 02	*M1
	0.5207E 01	0.2417E-02	-0.1001E-05	0.1879E-09	-0.1310E-13	-0.1833E 05	-0.2913E 01	*M2
CS	0.3398E 01	-0.5892E-03	0.5945E-05	-0.7086E-08	0.2616E-11	0.2648E 05	0.5919E 01	*M1
	0.3677E 01	0.9269E-03	-0.3887E-06	0.7439E-10	-0.5248E-14	0.2692E 05	0.3916E 01	*M2
CS2	0.2917E 01	0.1250E-01	-0.1611E-04	0.1057E-07	-0.2794E-11	0.1278E 05	0.8876E 01	*M1
	0.5949E 01	0.1724E-02	-0.7211E-06	0.1374E-09	-0.9684E-14	0.1205E 05	-0.6205E 01	*M2
C2	0.7509E 01	-0.1065E-01	0.1008E-04	-0.8621E-09	-0.1752E-11	0.9880E 05	-0.1608E 02	*M1
	0.4442E 01	-0.2885E-03	0.3036E-06	-0.6244E-10	0.3915E-14	0.9787E 05	-0.1090E 01	B2
	0.4026E 01	0.4857E-03	-0.7026E-07	0.4666E-11	-0.1142E-15	0.9787E 05	0.1090E 01	B3
C2H	0.3485E 01	0.3563E-02	-0.1237E-05	0.1866E-09	-0.1013E-13	0.5809E 05	0.4784E 01	B2
	0.5307E 01	0.8966E-03	-0.1378E-06	0.9251E-11	-0.2278E-15	0.5809E 05	-0.5288E 01	B3
C2H2	0.7903E 00	0.2347E-01	-0.3554E-04	0.2795E-07	-0.8448E-11	0.2625E 05	0.1401E 02	*M1
	0.3891E 01	0.5717E-02	-0.1957E-05	0.2931E-09	-0.1585E-13	0.2590E 05	0.6520E 00	B2
	0.6789E 01	0.1503E-02	-0.2295E-06	0.1534E-10	-0.3763E-15	0.2590E 05	-0.1539E 02	B3
C2H3	0.3486E 01	0.8263E-02	-0.2820E-05	0.4209E-09	-0.2268E-13	0.3140E 05	0.5278E 01	B2
	0.7538E 01	0.2298E-02	-0.3642E-06	0.2519E-10	-0.6378E-15	0.3140E 05	-0.1709E 02	B3
C2H4	0.1120E 01	0.1391E-01	0.2657E-05	-0.1156E-07	0.5239E-11	0.5333E 04	0.1584E 02	*M1
	0.2758E 01	0.1172E-01	-0.4053E-05	0.6098E-09	-0.3303E-13	0.6026E 04	0.7185E 01	B2
	0.8627E 01	0.3089E-02	-0.4864E-06	0.3342E-10	-0.8406E-15	0.6026E 04	-0.2516E 02	B3
C2H6	0.2382E 01	0.1032E-01	0.1191E-04	-0.1483E-07	0.4475E-11	-0.1162E 05	0.7598E 01	*D1
	0.1431E 01	0.1889E-01	-0.7044E-05	0.1187E-08	-0.7445E-13	-0.1143E 05	0.1401E 02	*D2

C2N2	0.3403E 01	0.1776E-01	-0.2686E-04	0.2197E-07	-0.7087E-11	0.3555E 05	0.5412E 01	*M1
	0.5396E 01	0.5089E-02	-0.1880E-05	0.2931E-09	-0.1620E-13	0.3563E 05	-0.2598E 01	B2
	-0.2697E 01	0.1308E-01	-0.3887E-05	0.4576E-09	-0.1878E-13	0.3563E 05	0.4498E 02	B3
C3	0.2633E 01	0.9419E-02	-0.9593E-05	0.5580E-08	-0.1424E-11	0.9431E 05	0.8079E 01	*M1
	0.4002E 01	0.3541E-02	-0.1318E-05	0.2064E-09	-0.1144E-13	0.9423E 05	0.2020E 01	B2
	0.2213E 02	-0.1759E-01	0.5565E-05	-0.6758E-09	0.2825E-13	0.9423E 05	-0.1021E 03	B3
C3H	0.2474E 01	0.1175E-01	-0.8045E-05	0.2729E-08	-0.3544E-12	0.6308E 05	0.1054E 02	*D1
C3H2	0.1668E 01	0.2219E-01	-0.2193E-04	0.1110E-07	-0.2153E-11	0.5230E 05	0.1304E 02	*D1
	0.4502E 01	0.8696E-02	-0.3154E-05	0.5242E-09	-0.3264E-13	0.5191E 05	0.1827E 00	*D2
C3H3	0.2588E 01	0.1891E-01	-0.1393E-04	0.5541E-08	-0.9975E-12	0.3700E 05	0.1032E 02	*D1
	0.4658E 01	0.1051E-01	-0.3955E-05	0.6723E-09	-0.4243E-13	0.3667E 05	0.6294E 00	*D2
C3H5	0.3159E 01	0.1511E-01	0.4407E-05	-0.9188E-08	0.2698E-11	0.1469E 05	0.1374E 02	*D1
	0.4153E 01	0.1671E-01	-0.6328E-05	0.1080E-08	-0.6880E-13	0.1439E 05	0.7926E 01	*D2
C3H8	0.2056E 01	0.2528E-01	-0.5914E-06	-0.6880E-08	0.3199E-11	-0.1426E 05	0.1318E 02	*D1
	0.1291E 01	0.2775E-01	-0.1047E-04	0.1781E-08	-0.1124E-12	-0.1407E 05	0.1715E 02	*D2
C4	0.5670E 01	0.5883E-02	-0.4751E-05	0.2349E-08	-0.4648E-12	0.1195E 06	-0.4253E 01	*D1
	0.6077E 01	0.3444E-02	-0.9480E-06	0.9348E-10	-0.1791E-14	0.1195E 06	-0.5995E 01	*D2
C4H	0.2696E 01	0.2268E-01	-0.2451E-04	0.1315E-07	-0.2673E-11	0.7649E 05	0.1040E 02	*D1
C4H2	0.6216E 01	0.9660E-02	-0.3489E-05	0.5411E-09	-0.2996E-13	0.5605E 05	-0.1211E 02	B2
	0.1118E 02	0.2194E-02	-0.3395E-06	0.2292E-10	-0.5670E-15	0.5605E 05	-0.3943E 02	B3

C4H3	0.5749E 01	0.1248E-01	-0.4751E-05	0.8136E-09	-0.5170E-13	0.4910E 05	-0.3430E 01 *D2
C5	0.7279E 01	0.6762E-02	-0.5026E-05	0.2562E-08	-0.5450E-12	0.1186E 06	-0.1311E 02 *D1
	0.7577E 01	0.4618E-02	-0.1271E-05	0.1188E-09	-0.1123E-14	0.1186E 06	-0.1431E 02 *D2
C5H	0.1022E 01	0.3109E-01	-0.3043E-04	0.1481E-07	-0.2783E-11	0.9217E 05	0.1757E 02 *D1
	0.5465E 01	0.1118E-01	-0.4300E-05	0.7241E-09	-0.4441E-13	0.9152E 05	-0.2844E 01 *D2
C5H2	0.1006E 01	0.4108E-01	-0.4555E-04	0.2475E-07	-0.5060E-11	0.8139E 05	0.1669E 02 *D1
	0.6655E 01	0.1325E-01	-0.5104E-05	0.8823E-09	-0.5645E-13	0.8063E 05	-0.8785E 01 *D2
C5H3	0.2649E 01	0.3462E-01	-0.3266E-04	0.1602E-07	-0.3088E-11	0.6608E 05	0.1140E 02 *D1
	0.7099E 01	0.1455E-01	-0.5664E-05	0.9844E-09	-0.6320E-13	0.6544E 05	-0.9039E 01 *D2
C5H6	0.8735E 00	0.2770E-01	0.4256E-05	-0.1440E-07	0.4466E-11	0.8995E 04	0.1905E 02 *D1
	0.3601E 01	0.2669E-01	-0.1037E-04	0.1800E-08	-0.1155E-12	0.8326E 04	0.4317E 01 *D2
C6	0.8888E 01	0.7644E-02	-0.5307E-05	0.2779E-08	-0.6265E-12	0.1437E 06	-0.1837E 02 *D1
	0.9077E 01	0.5792E-02	-0.1595E-05	0.1441E-09	-0.4628E-15	0.1437E 06	-0.1904E 02 *D2
C6H	0.2717E 01	0.3941E-01	-0.4505E-04	0.2477E-07	-0.5100E-11	0.1051E 06	0.1184E 02 *D1
	0.8362E 01	0.1165E-01	-0.4637E-05	0.8085E-09	-0.5150E-13	0.1043E 06	-0.1363E 02 *D2
C6H2	0.2324E 01	0.4630E-01	-0.5461E-04	0.3087E-07	-0.6480E-11	0.8307E 05	0.1082E 02 *D1
	0.8775E 01	0.1341E-01	-0.5232E-05	0.9113E-09	-0.5860E-13	0.8223E 05	-0.1805E 02 *D2
C6H3	0.2926E 01	0.4065E-01	-0.3887E-04	0.1907E-07	-0.3666E-11	0.7738E 05	0.1118E 02 *D1
	0.8313E 01	0.1640E-01	-0.6416E-05	0.1119E-08	-0.7200E-13	0.7660E 05	-0.1357E 02 *D2
C6H6	0.3511E 00	0.3754E-01	-0.7947E-05	-0.7509E-08	0.3038E-11	0.8264E 04	0.1987E 02 *D1
	0.4620E 01	0.2881E-01	-0.1124E-04	0.1958E-08	-0.1257E-12	0.7392E 04	-0.1789E 01 *D2

C7	0.1050E 02	0.8524E-02	-0.5585E-05	0.2994E-08	-0.7075E-12	0.1436E 06 -0.2722E 02 *D1
	0.1058E 02	0.6963E-02	-0.1917E-05	0.1689E-09	0.2555E-15	0.1436E 06 -0.2736E 02 *M2
C7H	0.1744E 01	0.4949E-01	-0.5613E-04	0.3040E-07	-0.6175E-11	0.1194E 06 0.1562E 02 *D1
	0.9024E 01	0.1425E-01	-0.5734E-05	0.1009E-08	-0.6475E-13	0.1184E 06 -0.1734E 02 *D2
C7H2	0.2030E 01	0.4776E-01	-0.5111E-04	0.2777E-07	-0.5745E-11	0.1088E 06 0.1366E 02 *D1
	0.8139E 01	0.1758E-01	-0.6763E-05	0.1167E-08	-0.7450E-13	0.1080E 06 -0.1389E 02 *D2
C8	0.1211E 02	0.9404E-02	-0.5861E-05	0.3208E-08	-0.7885E-12	0.1696E 06 -0.3249E 02 *D1
	0.1209E 02	0.8134E-02	-0.2238E-05	0.1935E-09	0.9902E-15	0.1696E 06 -0.3210E 02 *D2
C8H	0.1532E 01	0.5652E-01	-0.6394E-04	0.3473E-07	-0.7085E-11	0.4291E 05 0.6400E-01 *D1
	0.9773E 01	0.1663E-01	-0.8198E-05	0.1181E-08	-0.7600E-13	0.1418E 06 -0.2084E 02 *D2
C8H2	0.1087E 01	0.6487E-01	-0.7572E-04	0.4207E-07	-0.8700E-11	0.1112E 06 0.1567E 02 *D1
	0.1047E 02	0.1820E-01	-0.7243E-05	0.1278E-08	-0.8285E-13	0.1100E 06 -0.2657E 02 *D2
C9	0.1371E 02	0.1029E-01	-0.6144E-05	0.3427E-08	-0.8705E-12	0.1670E 06 -0.4134E 02 *D1
	0.1358E 02	0.9308E-02	-0.2562E-05	0.2189E-09	0.1542E-14	0.1670E 06 -0.4041E 02 *D2
C9H	0.1099E 01	0.6769E-01	-0.7887E-04	0.4345E-07	-0.8925E-11	0.1448E 06 0.1813E 02 *D1
	0.1114E 02	0.1843E-01	-0.7453E-05	0.1318E-08	-0.8510E-13	0.1434E 00 -0.2008E 00 *D2
C9H2	0.1692E 01	0.6336E-01	-0.7042E-04	0.3834E-07	-0.7975E-11	0.1342E 06 0.1499E 02 *D1
	0.1006E 02	0.2136E-01	-0.8502E-05	0.1477E-08	-0.9480E-13	0.1331E 06 -0.2275E 02 *D2
C10	0.1532E 02	0.1117E-01	-0.6422E-05	0.3642E-08	-0.9510E-12	0.1965E 06 -0.4661E 02 *D1
	0.1503E 02	0.1048E-01	-0.2805E-05	0.2439E-09	0.2339E-14	0.1966E 06 -0.4514E 02 *D2

C10H	0.2248E 01	0.7022E-01	-0.8037E-04	0.4395E-07	-0.9005E-11	0.1714E 06	0.1442E 02	*D1
	0.1255E 02	0.2011E-02	-0.8136E-05	0.1440E-08	-0.9305E-13	0.1708E 06	-0.2678E 02	*D2
C10H2	0.1810E 01	0.7857E-01	-0.9245E-04	0.5162E-07	-0.1072E-10	0.1396E 06	0.1360E 02	*D1
	0.1322E 02	0.2166E-01	-0.8660E-05	0.1532E-08	-0.9955E-13	0.1361E 06	-0.3773E 02	*D2
E-	0.2500E 01	0.3440E-06	-0.1954E-09	0.3937E-13	-0.2573E-17	-0.7450E 03	-0.1173E 02	B2
	0.2503E 01	-0.6332E-05	0.1364E-08	-0.1094E-12	0.2934E-17	-0.7450E 03	-0.1208E 02	B3
H	0.2500E 01	0.0	0.0	0.0	0.0	0.2547E 05	-0.4600E 00	*M1
	0.2500E 01	-0.8243E-05	0.6421E-09	-0.1720E-12	0.1457E-16	0.2547E 05	-0.4612E 00	B2
	0.3934E 01	-0.1776E-02	0.6013E-06	-0.7819E-10	0.3482E-14	0.2547E 05	-0.8598E 01	B3
HCN	0.2168E 01	0.1073E-01	-0.1509E-04	0.1193E-07	-0.3700E-11	0.1468E 05	0.9281E 01	*M1
	0.3654E 01	0.3444E-02	-0.1258E-05	0.2169E-09	-0.1430E-13	0.1442E 05	0.2373E 01	*M2
	0.3654E 01	0.3444E-02	-0.1258E-05	0.2169E-09	-0.1430E-13	0.1442E 05	0.2373E 01	*M3
HCO+	0.3463E 01	0.3155E-02	-0.1091E-05	0.1636E-09	-0.8836E-14	0.1027E 06	0.6279E 01	B2
	0.5093E 01	0.7856E-03	-0.1212E-06	0.8161E-11	-0.2013E-15	0.1027E 06	-0.2739E 01	B3
HCO	0.3865E 01	-0.5371E-03	0.6903E-05	-0.6645E-08	0.2058E-11	-0.2800E 04	0.4897E 01	*M1
	0.3503E 01	0.3025E-02	-0.1004E-05	0.1444E-09	-0.7512E-14	-0.2824E 04	0.6061E 01	B2
	0.5093E 01	0.7856E-03	-0.1212E-06	0.8161E-11	-0.2013E-15	-0.2824E 04	-0.2739E 01	B3
HO2	0.3632E 01	0.2849E-02	-0.9587E-06	0.1417E-09	-0.7590E-14	0.1326E 04	0.5119E 01	B2
	0.5071E 01	0.7800E-03	-0.1191E-06	0.7957E-11	-0.1952E-15	0.1326E 04	-0.2862E 01	B3
HS	0.4259E 01	-0.1278E-02	-0.8379E-06	0.3832E-08	-0.2025E-11	0.1702E 05	-0.3537E 00	*M1
	0.2988E 01	0.1359E-02	-0.4711E-06	0.7904E-10	-0.5058E-14	0.1739E 05	0.6348E 01	*M2

H2	0.2846E 01	0.4193E-02	-0.9612E-05	0.9512E-08	-0.3309E-11	-0.9673E 03	-0.1412E 01	*M1
	0.3358E 01	0.2794E-03	0.9372E-07	-0.2948E-10	0.2141E-14	-0.1018E 04	-0.3548E 01	B2
	0.3363E 01	0.4656E-03	-0.5127E-07	0.2802E-11	-0.4905E-16	-0.1018E 04	-0.3716E 01	B3
H2CO	0.2908E 01	0.6323E-02	-0.2188E-05	0.3284E-09	-0.1775E-13	-0.2605E 04	0.7722E 01	B2
	0.6181E 01	0.1566E-02	-0.2407E-06	0.1614E-10	-0.3966E-15	-0.2605E 04	-0.1039E 02	B3
H2O	0.4156E 01	-0.1724E-02	0.5698E-05	-0.4593E-08	0.1423E-11	-0.3029E 05	-0.6862E 00	*M1
	0.3387E 01	0.2140E-02	-0.5048E-06	0.5269E-10	-0.1999E-14	-0.3028E 05	0.2635E 01	B2
	0.4339E 01	0.1039E-02	-0.1545E-06	0.1017E-10	-0.2468E-15	-0.3028E 05	-0.2837E 01	B3
H3O+	0.2934E 01	0.4980E-02	-0.1438E-05	0.1882E-09	-0.9155E-14	0.6955E 05	0.4949E 01	B2
	0.5321E 01	0.1848E-02	-0.2780E-06	0.1839E-10	-0.4476E-15	0.6955E 05	-0.8500E 01	B3
H2S	0.3916E 01	-0.3514E-03	0.4219E-05	-0.2745E-08	0.4858E-12	-0.3609E 04	0.2366E 01	*M1
	0.2766E 01	0.4013E-02	-0.1504E-05	0.2681E-09	-0.1797E-13	-0.3386E 04	0.7932E 01	*M2
N+	0.2727E 01	-0.2820E-03	0.1105E-06	-0.1551E-10	0.7847E-15	0.2254E 06	0.3645E 01	B2
	0.2499E 01	-0.3725E-05	0.1147E-07	-0.1102E-11	0.3078E-16	0.2254E 06	0.4950E 01	B3
N++	0.2775E 01	-0.3385E-03	0.1408E-06	-0.2374E-10	0.1387E-14	0.4557E 06	0.2946E 01	B2
	0.2559E 01	-0.6470E-05	-0.2512E-08	0.3786E-12	-0.8326E-17	0.4557E 06	0.4136E 01	B3
N+++	0.2500E 01	-0.4722E-06	0.3938E-09	-0.1124E-12	0.1016E-16	0.1008E 07	0.2794E 01	B2
	0.2404E 01	0.8766E-04	-0.2049E-07	0.1624E-11	-0.3008E-16	0.1008E 07	0.3369E 01	B3
N	0.2515E 01	-0.1124E-03	0.2965E-06	-0.3246E-09	0.1259E-12	0.5613E 05	0.4119E 01	*M1
	0.2474E 01	0.9097E-04	-0.7814E-07	0.2218E-10	-0.1489E-14	0.5609E 05	0.4300E 01	B2
	0.2746E 01	-0.3909E-03	0.1338E-06	-0.1191E-10	0.3369E-15	0.5609E 05	0.2872E 01	B3

NH	0.3455E 01	0.5280E-03	-0.1973E-05	0.2958E-08	-0.1208E-11	0.3867E 05	0.2010E 01	*M1
	0.2727E 01	0.1420E-02	-0.4583E-06	0.7555E-10	-0.4617E-14	0.3893E 05	0.6044E 01	*M2
NH3	0.3772E 01	-0.4862E-03	0.9874E-05	-0.9568E-08	0.3131E-11	-0.6728E 04	0.1465E 01	*M1
	0.2149E 01	0.6493E-02	-0.2269E-05	0.3739E-09	-0.2361E-13	-0.6401E 04	0.9820E 05	*M2
NO+	0.3200E 01	0.1029E-02	-0.3075E-06	0.4028E-10	-0.1814E-14	0.1184E 06	0.5225E 01	B2
	0.3561E 01	0.6028E-03	-0.1540E-06	0.1697E-10	-0.5296E-15	0.1184E 06	0.3170E 01	B3
NO	0.4147E 01	-0.4126E-02	0.9692E-05	-0.7863E-08	0.2231E-11	0.9745E 04	0.2569E 01	*M1
	0.3221E 01	0.1221E-02	-0.4297E-06	0.6559E-10	-0.3451E-14	0.9764E 04	0.6610E 01	B2
	0.3845E 01	0.2521E-03	-0.2658E-07	0.2162E-11	-0.6381E-16	0.9764E 04	0.3212E 01	B3
NO2	0.3434E 01	0.2223E-02	0.6715E-05	-0.9743E-08	0.3721E-11	0.2865E 04	0.8408E 01	*M1
	0.4614E 01	0.2639E-02	-0.1095E-05	0.2082E-09	-0.1465E-13	0.2340E 04	0.1368E 01	*M2
NS	0.4062E 01	-0.2819E-02	0.9316E-05	-0.9509E-08	0.3284E-11	0.3087E 05	0.4061E 01	*M1
	0.3840E 01	0.7457E-03	-0.3058E-06	0.5805E-10	-0.4069E-14	0.3079E 05	0.4472E 01	*M2
N2+	0.3397E 01	0.4525E-03	0.1272E-06	-0.3879E-10	0.2459E-14	0.1826E 06	0.4205E 01	B2
	0.3370E 01	0.8629E-03	-0.1276E-06	0.8087E-11	-0.1880E-15	0.1826E 06	0.4073E 01	B3
N2	0.3692E 01	-0.1333E-02	0.2650E-05	-0.9769E-09	-0.9977E-13	-0.1063E 04	0.2287E 01	*M1
	0.3221E 01	0.9878E-03	-0.2907E-06	0.3938E-10	-0.2000E-14	-0.1043E 04	0.4326E 01	B2
	0.3727E 01	0.4684E-03	-0.1140E-06	0.1154E-10	-0.3293E-15	-0.1043E 04	0.1294E 01	B3
N2O	0.2382E 01	0.1035E-01	-0.1117E-04	0.6958E-08	-0.1878E-11	0.8723E 04	0.1023E 02	*M1
	0.4627E 01	0.3022E-02	-0.1216E-05	0.2286E-09	-0.1585E-13	0.8136E 04	-0.1146E 01	*M2
N2O4	0.3165E 01	0.2719E-01	-0.2535E-04	0.1099E-07	-0.1660E-11	-0.7673E 03	0.1148E 02	*M1
	0.1043E 01	0.6036E-02	-0.2583E-05	0.4928E-09	-0.3478E-13	-0.2741E 04	-0.2582E 02	*M2

NE+	0.2705E 01	-0.9724E-04	0.1205E-07	0.5333E-12	-0.1213E-15	0.2252E 06	0.3716E 01	B2
	0.2664E 01	-0.6497E-04	0.9630E-08	-0.6142E-12	0.1413E-16	0.2252E 06	0.3961E 01	B3
NE++	0.2818E 01	-0.2139E-03	0.5385E-07	-0.5739E-11	0.2467E-15	0.7276E 06	0.3424E 01	B2
	0.2787E 01	-0.1600E-03	0.3031E-07	-0.1952E-11	0.4256E-16	0.7276E 06	0.3588E 01	B3
NE+++	0.2501E 01	-0.2586E-05	0.2462E-08	-0.8359E-12	0.9277E-16	0.1468E 07	0.4726E 01	B2
	0.2505E 01	0.1709E-04	-0.1147E-07	0.1808E-11	-0.5856E-16	0.1468E 07	0.4681E 01	B3
NE	0.2500E 01	0.9686E-06	-0.5972E-09	0.1288E-12	-0.8901E-17	-0.7454E 03	0.3684E 01	B2
	0.2571E 01	-0.6481E-04	0.1585E-07	-0.1469E-11	0.4619E-16	-0.7454E 03	0.2918E 01	B3
O+	0.2491E 01	0.2762E-04	-0.1881E-07	0.3807E-11	-0.1028E-15	0.1879E 06	0.4424E 01	B2
	0.2944E 01	-0.4108E-03	0.9156E-07	-0.5848E-11	0.1190E-15	0.1879E 06	0.1750E 01	B3
O++	0.2983E 01	-0.5800E-03	0.2334E-06	-0.3768E-10	0.2168E-14	0.5961E 06	0.2307E 01	B2
	0.2706E 01	-0.1315E-03	0.3048E-07	-0.2207E-11	0.5305E-16	0.5961E 06	0.3812E 01	B3
O+++	0.3015E 01	-0.5885E-03	0.2355E-06	-0.3875E-10	0.2226E-14	0.1234E 07	0.1668E 01	B2
	0.2683E 01	-0.7049E-04	0.9853E-08	-0.6203E-12	0.1678E-16	0.1234E 07	0.3482E 01	B3
O	0.3022E 01	-0.2174E-02	0.3754E-05	-0.2995E-08	0.9078E-12	0.2914E 05	0.2646E 01	*M1
	0.2670E 01	-0.1970E-03	0.7193E-07	-0.8901E-11	0.4002E-15	0.2915E 05	0.4504E 01	B2
	0.2548E 01	-0.5952E-04	0.2701E-07	-0.2798E-11	0.9380E-16	0.2915E 05	0.5049E 01	B3
O-	0.2500E 01	0.3440E-06	-0.1954E-09	0.3937E-13	-0.2573E-17	0.1141E 05	0.4786E 01	B2
	0.2508E 01	-0.6332E-05	0.1364E-08	-0.1094E-12	0.2934E-17	0.1141E 05	0.4739E 01	B3
OH	0.3823E 01	-0.1119E-02	0.1247E-05	-0.2104E-09	-0.5255E-13	0.3585E 04	0.5825E 00	*M1
	0.3284E 01	0.5087E-03	-0.2289E-07	-0.1001E-10	0.1056E-14	0.3626E 04	0.3232E 01	B2
	0.3456E 01	0.4375E-03	-0.5819E-07	0.4187E-11	-0.1104E-15	0.3626E 04	0.2149E 01	B3

O2+	0.3243E 01	0.1174E-02	-0.3900E-06	0.5437E-10	-0.2392E-14	0.1400E 06	0.5925E 01	B2
	0.5169E 01	-0.8620E-03	0.2041E-06	-0.1300E-10	0.2494E-15	0.1400E 06	-0.5296E 01	B3
O2	0.3719E 01	-0.2517E-02	0.8584E-05	-0.8300E-08	0.2708E-11	-0.1058E 04	0.3908E 01	*M1
	0.3316E 01	0.1151E-02	-0.3726E-06	0.6186E-10	-0.3666E-14	-0.1044E 04	0.5393E 01	B2
	0.3721E 01	0.4254E-03	-0.2835E-07	0.6050E-12	-0.5186E-17	-0.1044E 04	0.3254E 01	B3
O2-	0.3402E 01	0.1243E-02	-0.5081E-06	0.9982E-10	-0.6398E-14	-0.1063E 05	0.5428E 01	B2
	0.3648E 01	0.2944E-03	0.5360E-07	-0.8789E-11	0.2828E-15	-0.1063E 05	0.4575E 01	B3

APPENDIX B

DETERMINATION OF THE HEATS OF FORMATION OF PURE COMPOUNDS AT 298°K

As indicated in the introduction of this report, several sources used for the thermodynamic functions gave tabulated properties of enthalpy and free energy relative to elements at 0°K. In order to transform this reference temperature to 298.16, it is necessary to know the heat of reaction at the latter temperature. The method used can be best illustrated by Figure B-1.

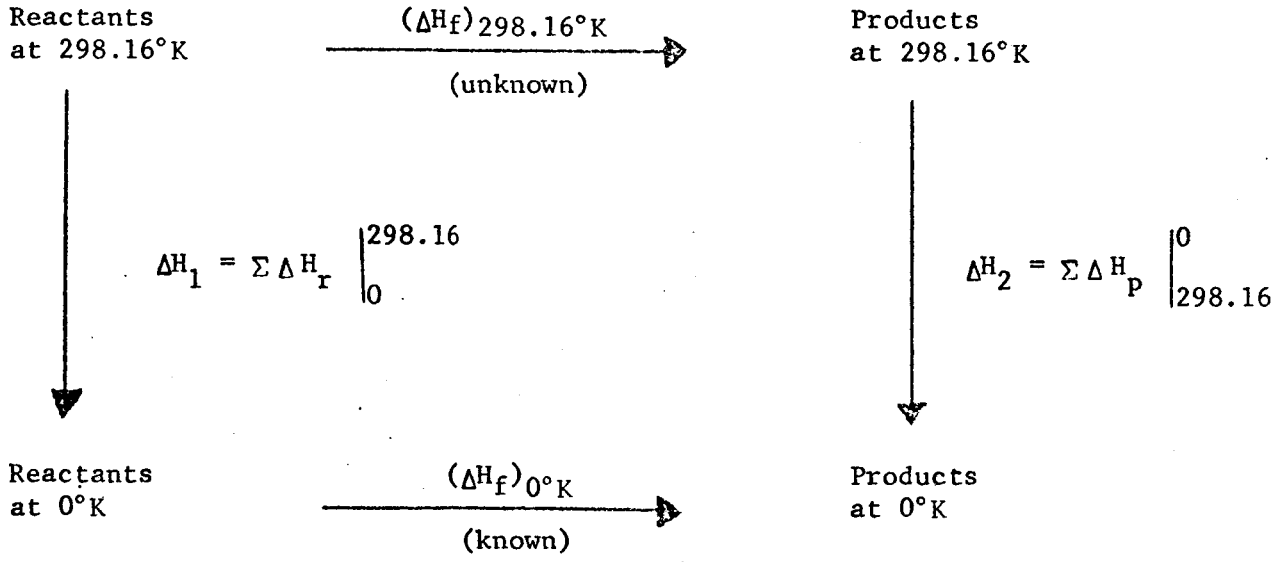

Figure B-1. Determination of Heat of Formation at 298.16°K from Heat of Formation at 0°K

By definition, the heat of formation of a compound is the enthalpy change incurred by its production. Since enthalpy is a point function and as such is independent of path, we can cool the reactants from the reference temperature of 0°K, allow the formation reaction to occur at the lower temperature, and then heat the products back to the new reference temperature of 298.16°K. Through this process we can establish the enthalpy of

the reaction products relative to the reactants or the heat of reaction at 298.16 by the following relation,

$$(\Delta H_f^\circ)_{298.16} = (\Delta H_f^\circ)_0 + \Delta H_1 + \Delta H_2 \qquad \text{(B-1)}$$

Some care must be exercised in selecting the reaction for the formation of a particular compound. The enthalpy of the reactants must be specified relative to the reference species. It is therefore convenient to use the reference species as reactants in formation reaction. The reference elements used in this analysis are; H_2, N_2, O_2, Ne, Ar, He, carbon solid and e^-. The reaction used for the formation of each compound are listed in Table B-1. Also included in this table are the heats of formation at 0°K and 298.16°K.

Table B-1. Reactions and Heats of Formation

Component	Reaction	$(\Delta H_f^\circ)_{298.16}$ (Kcal/gmole)	$(\Delta H_f^\circ)_0$ (Kcal/gmole)	Reference
N	$1/2\ N_2 \rightarrow N$	112.951	112.507	2
O	$1/2\ O_2 \rightarrow O$	59.544	58.972	2
C(gas)	$C \rightarrow C$	171.301	169.990	2
A^+	$A \rightarrow A^+ + e^-$	364.828	363.345	2
N^+	$1/2\ N_2 \rightarrow N^+ + e^-$	449.709	447.564	2
O^+	$1/2\ O_2 \rightarrow O^+ + e^-$	374.867	372.942	2
C^+	$C_s \rightarrow C^+ + e^-$	432.357	429.537	2
Ne^+	$Ne \rightarrow Ne^+ + e^-$	449.071	497.186	2
A^{++}	$A \rightarrow A^{++} + 2e^-$	1003.252	1000.280	2
N^{++}	$1/2\ N_2 \rightarrow N^{++} + 2e^-$	907.179	905.023	2
O^{++}	$1/2\ O_2 \rightarrow O^{++} + 2e^-$	1186.408	1182.600	2
C^{++}	$C_s \rightarrow C^{++} + 2e^-$	995.898	991.689	2
Ne^{++}	$Ne \rightarrow Ne^{++} + 2e^-$	1447.366	1444.350	2
A^{+++}	$A \rightarrow A^{+++} + 3e^-$	1947.934	1943.490	2
N^{+++}	$1/2\ N_2 \rightarrow N^{+++} + 3e^-$	2003.648	1998.760	2
O^{+++}	$1/2\ O_2 \rightarrow O^{+++} + 3e^-$	2454.520	2449.470	2
C^{+++}	$C_s \rightarrow C^{+++} + 3e^-$	2101.403	2095.690	2
Ne^{+++}	$Ne \rightarrow Ne^{+++} + 3e^-$	2918.493	2914.050	2
O^-	$1/2\ O_2 + e^- \rightarrow O^-$	24.156	25.193	2
H	$1/2\ H_2 \rightarrow H$	52.098	51.620	5
OH	$1/2\ O_2 + 1/2\ H_2 \rightarrow OH$	9.3575	9.300	5
H_2O	$1/2\ O_2 + H_2 \rightarrow H_2O$	-57.8018	-57.107	5
HO_2	$O_2 + 1/2\ H_2 \rightarrow HO_2$	5.0244	5.700	5
HCO	$C_2 + 1/2\ O_2 + 1/2\ H_2 \rightarrow HCO$	-3.224	-3.311	9
H_2CO	$C_s + 1/2\ O_2 + H_2 \rightarrow H_2\ CO$	-27.8168	-26.900	5
HCO^+	$C_s + 1/2\ O_2 + 1/2\ H_2 \rightarrow HCO^+ + e^-$	206.5688	205.000	5
H_3O^+	$O_2 + 3H_2 \rightarrow 2H_3O^+ + 2e^-$	140.6009	141.000	5
C_2	$C_s \rightarrow C_2$	197.0259	195.000	5
CH	$C_s + 1/2\ H_2 \rightarrow CH$	142.3965	141.600	5
CH_2	$C_s + H_2 \rightarrow CH_2$	94.8097	95.000	5
CH_3	$2C_s + 3H_2 \rightarrow 2CH_3$	31.8032	34.400	5
CH_4	$C_s + 2H_2 \rightarrow CH_4$	-17.8964	-15.990	5

Table B-1. (cont.)

Component	Reaction	$(\Delta H_f^\circ)_{298.16}$ (Kcal/gmole)	$(\Delta H_f^\circ)_0$ (Kcal/gmole)	Reference
C_2H	$2C_s + 1/2\ H_2 \rightarrow C_2H$	117.6488	116.700	5
C_2H_2	$2C_s + H_2 \rightarrow C_2H_2$	53.8670	54.330	5
C_2H_3	$4C_s + 3H_2 \rightarrow 2C_2H_3$	64.9850	66.900	5
C_2H_4	$2C_s + 2H_2 \rightarrow C_2H_4$	14.4926	14.520	5
C_4H_2	$4C_s + H_2 \rightarrow C_4H_2$	111.7205	111.300	5
NO	$1/2\ N_2 + 1/2\ O_2 \rightarrow NO$	21.6009	21.477	3
CO	$C_s + 1/2\ O_2 \rightarrow CO$	-26.4179	-27.202	3
O_2^+	$O_2 \rightarrow O_2^+ + e^-$	280.2099	277.918	3
N_2^+	$N_2 \rightarrow N_2^+ + e^-$	364.9392	359.306	3
NO^+	$1/2\ N_2 + 1/2\ O_2 \rightarrow NO^+ + e^-$	237.3239	235.836	3
CO^+	$C_s + 1/2\ O_2 \rightarrow CO^+ + e^-$	298.2493	295.977	3
O_2^-	$e^- + O_2 \rightarrow O_2^-$	-19.0502	-23.000	3
CN	$C_s + 1/2\ N_2 \rightarrow CN$	109.7865	109.000	4
C_2N_2	$2C_s + N_2 \rightarrow C_2N_2$	74.1277	73.400	4
C_3	$3C_s \rightarrow C_3$	189.6115	188.000	4
C^-	$C_s + e^- \rightarrow C^-$	142.2300	141.000	4

APPENDIX C

LISTING OF COMPUTER PROGRAM

```
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
C          PROGRAM FOR CURVE-FIT OF THERMODYNAMIC FUNCTIONS              *
C                                                                        *
C     THIS PROGRAM CALCULATES THE VALUES OF THE CONSTANTS A1-A7 FOR      *
C     THE POLYNOMIAL FORMS OF THE FREE ENERGY, ENTHALPY, HEAT            *
C     CAPACITY, AND ENTROPY RELATIONSHIPS AS USED IN MCBRIDE,ET AL.,     *
C     NASA SP-3001, PP. 14-15.                                           *
C                                                                        *
C     THE FOLLOWING INPUT DATA ARE REQUIRED*                             *
C                                                                        *
C            1.  IDENTIFICATION CARD-- CONSISTS OF SPECIES               *
C                NAME IN COLS. 1-8, REFERENCE TEMPERATURE                *
C                IN COLS. 16-22, DELTA H OF FORMATION AT THE             *
C                REFERENCE TEMPERATURE (CAL/MOLE) IN COLS. 32-46,        *
C                AND THE VALUE OF THE ENTHALPY FUNCTION AT THE           *
C                REFERENCE TEMPERATURE (CAL/MOLE) IN COLS. 51-60.        *
C                ALL NUMERICAL ENTRIES ON THIS CARD ARE TO BE IN         *
C                F-FORMAT.                                               *
C            2.  SOURCE CARD -- COLS.1-79 ARE AVAILABLE                  *
C                FOR A BRIEF BIBLIOGRAPHICAL CITATION.                   *
C            3.  FUNCTION DATA CARDS -- THESE CARDS CONTAIN              *
C                TEMPERATURES IN COLS. 1-6, AND THE                      *
C                CORRESPONDING VALUES OF THE FREE ENERGY                 *
C                AND ENTHALPY FUNCTIONS RESPECTIVELY IN                  *
C                COLS 7-20 AND 21-34.  THE FORM OF THESE                 *
C                FUNCTIONS AS REQUIRED FOR INPUT CAN BE VARIED.          *
C                IN GENERAL, TABULATED DATA IS OF THE FORM OF            *
C                -(F-H*)/T. IF THE DATA IS OF THE FORM OF -(F-H*),       *
C                THE NUMBER 1 CAN BE INSERTED IN COL. 80 OF              *
C                THE SOURCE CARD AND THE INPUT WILL BE TRANSFORMED       *
C                INTERNALLY TO THE GENERAL FORM.
C            4.  TERMINATION CARD--A NEGATIVE VALUE IN COLS. 1-6         *
C                WILL TERMINATE DATA INPUT. AFTER THIS PACKAGE HAS       *
C                HAS BEEN PROCESSED A NEW SET OF CARDS WILL BE READ.     *
C                                                                        *
C                                                                        *
C                                        DONALD D. ESCH                  *
C                                        LOUISIANA STATE UNIVERSITY      *
C                                        AUGUST 1970                     *
C * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
001          DOUBLE PRECISION T(100),H(100),B(7)
002          DIMENSION SOURCE(39),SP(2),F(100),HC(100),FC(100),A(7)
003          DIMENSION S(100),CP(100),HH(100)
004          INTEGER RANGE
005          R=1.98718
006       10 I=1
007          READ 100,SP,TRER,DELH,HREF
008          READ 101,SOURCE,NTYPE
009       20 READ 102,T(I),F(I),H(I)
010          IF(T(I).LT.0.0)GOTO30
011          I=I+1
012          GOTO20
013       30 NUMBER=I-1
014          TREF=298.16
C
C-----SET UP ARRAYS FOR LEAST SQUARES FIT.
C
015          DO50I=1,NUMBER
```

```
016                H(I)=H(I)/R
017          50    F(I)=-F(I)/R
018                IF(NTYPE.EQ.0)GOTO70
019                DO60I=1,NUMBER
020                H(I)=H(I)/T(I)
021          60    F(I)=F(I)/T(I)
022          70    CONTINUE
             C
023                CALL LSFIT(T,H,NUMBER,4,B)
             C
024                A(1)=B(1)
025                A(2)=B(2)*2.
026                A(3)=B(3)*3.
027                A(4)=B(4)*4.
028                A(5)=B(5)*5.
             C
             C-----DETERMINE THE VALUE OF A(6)
             C
029                HZERO=DELH-HREF
030                A(6)=HZERO/R
             C
             C-----DETERMINE THE VALUE OF A(7)
             C
031                SUMA7=0.0
032                DO80I=1,NUMBER
033                TEMP=T(I)
034                FEST=A(1)*(1.-ALOG(TEMP))-A(2)*T(I)/2.-A(3)*(T(I)**2)/6.-A(4)*
                  1 (T(I)**3)/12. -A(5)*(T(I)**4)/20.
035                DF=FEST-F(I)
036          80    SUMA7=SUMA7+DF
037                A(7)=SUMA7/NUMBER
             C
             C-----DETERMINE TEMPERATURE RANGE---RANGE 1 INCLUDE TEMPERATURES FROM
             C     0 TO 1000, RANGE 2 FROM 1000 TO 6000, AND RANGE 3 FROM 6000 TO
             C     18000 DEGREES KELVIN.
             C
038                RANGE=1
039                IF(T(NUMBER).LE.1000)GOTO85
040                RANGE=2
041                IF(T(NUMBER).LE.8000)GOTO85
042                RANGE=3
043          85    CONTINUE
             C
             C-----OUTPUT
             C
             C-----PUNCH OUT THERMO DATA CARDS FOR CHEMEQ PROGRAM
             C
             C     DO88N=1,20
             C88   WRITE(7,117)(A(I),I=1,7),SP,RANGE
             C
044                PRINT 113
045                PRINT 103,SP
046                IF (RANGE.LT.3)GOTO47
047                IF (T(NUMBER).EQ.10000) GO TO 51
048                ITLO=6000
049                ITHI=15000
050                JANE=6
051                JIM=24
```

```
RTRAN IV G LEVEL  18                MAIN                DATE = 71062          18/05/46

052               GO TO 49
053            51 ITLO=6000
054               ITHI=10000
055               JANE=6
056               JIM=26
057
058               GOTO49


059            47 ITLO=1000
060               ITHI=6000
061               JANE=1
062               JIM=26
063            49 PRINT 104,ITLO,ITHI
064               PRINT 105,TREF
065               PRINT 106
066               PRINT 108
067               DO90I=JANE,JIM
068               TEMP=T(I)
069               FC(I)=A(1)*(1.-ALOG(TEMP))-A(2)*T(I)/2.-A(3)*(T(I)**2)/6.
                 1     -A(4)*(T(I)**3)/12. - A(5)*(T(I)**4)/20. - A(7)
070               FC(I)=-FC(I)
071               HC(I)=A(1) + A(2)*T(I)/2. + A(3)*(T(I)**2)/3. + A(4)*(T(I)**3)/4.
                 1  + A(5)*(T(I)**4)/5.
072               CP(I)=A(1) + A(2)*T(I) + A(3)*(T(I)**2) + A(4)*(T(I)**3)    +
                 &  A(5)*(T(I)**4)
073               S(I)=A(1)*ALOG(TEMP) + A(2)*T(I) + A(3)*(T(I)**2)/2.
                 &    + A(4)*(T(I)**3)/3. + A(5)*(T(I)**4)/4. + A(7)
074               HTO=HC(I) + (A(6)/T(I))
075               NT=T(I)
076            90 PRINT 112,NT,FC(I),HC(I),S(I),CP(I),HTO
077               PRINT 108
078               PRINT 109
079               PRINT 110,(A(I),I=1,7)
080               PRINT 111,SOURCE
081               NN=JIM-JANE
082               NCOUNT=26-NN
083               IF(NCOUNT.LT.1)NCOUNT=1
084               DO95N=1,NCOUNT
085            95    PRINT 116
086                  PRINT 114
087                  WRITE(6,117)(A(I),I=1,7),SP,RANGE
088                  PRINT 115
089                  GOTO10
090            200   STOP
               C
               C----- F O R M A T   S T A T E M E N T S
               C
091             100  FORMAT(2A3,9X,F6.2,10X,F14.5,5X,F10.2)
092             101  FORMAT(39A2,I2)
093             102  FORMAT(F6.0,2E14.4)
094             103  FORMAT(25X,'POLYNOMIAL CONSTANTS AND THERMODYNAMIC PROPERTIES OF '
                    1 ,2A3)
095             104  FORMAT(25X,'OVER A TEMPERATURE RANGE OF ',I5,' TO ',I5,' DEGREES K
                    1ELVIN.')
096             105  FORMAT(37X,'REFERENCE TEMPERATURE = ',F6.2,//)
097              106 FORMAT (14X,'T(K)',5X,'-(F-H*)/RT',7X,'(H-H*)/RT',10X,'S/R',13X,'C
                    1P/R',11X,'H/RT')
```

```
RTRAN IV G LEVEL  18                    MAIN                    DATE = 71062          18/05/4

098          108  FORMAT(10X,18('-----'),/)
099          109  FORMAT(                16X,'A1',11X,'A2',11X,'A3',11X,'A4',11X,'A5',
                 1 11X,'A6',11X,'A7')
100          110  FORMAT(10X,7(E13.6),/)
101          111  FORMAT(8X,' SOURCE OF DATA* ',5X,3(A2))
102          112  FORMAT(10X,I8,5E16.6)
103          113  FORMAT(1H1,/,22('-----'),7(/,' ',108X,' '))
104          114  FORMAT(       22('-----'))
105          115  FORMAT(1H1)
106          116  FORMAT(' ',108X,' ')
107          117  FORMAT(7E10.4,2X,2A3,1X,I1)
108           120 FORMAT(F20.2)
109               END
```

```
IRTRAN IV G LEVEL  18                    LSFIT                    DATE = 71062          18/05/46

001                SUBROUTINE LSFIT(X,Y,NUMBER,M,C)
                C
                C
                C     LEAST SQUARE CURVE FITTING OF ANY ORDER POLYNOMIAL
                C     OF ORDER EQUAL TO OR LESS THAN 10
                C
                C
                C
                C     NUMBER    IS THE ACTUAL NUMBER OF X-Y DATA PAIRS.,MAXIMUM OF 200
                C     M IS THE DEGREE OF THE POLYNOMIAL.,MAXIMUM OF 10
                C     N IS THE NUMBER OF EQUATIONS(=M+1)
                C     X,Y IS THE ARRAY FOR THE DATA PAIRS
                C     A IS THE ARRAY FOR THE SUM, WHICH BECOME THE COEFFICIENTS OF THE
                C     UNKNOWN IN THE SIMULTANEOUS EQUATIONS.
                C     B IS THE ARRAY FOR THE CONSTANT TERMS IN THE SIMULTANEOUS EQUATIONS
                C     C IS THE ARRAY FOR THE UNKNOWNS, WHICH BECOME THE COEFFICIENS IN
                C     THE POLYNOMIAL.
                C     P IS THE ARRAY FOR THE POWERS OF THE X(I),FROM 1 TO 2M.
                C
002                REAL*8             X(100),Y(100),A(7,7),B(7),C(7),P(20)
                C
003                MX2=M*2
004                DO 13 I=1,MX2
005                P(I)=0.0
006                DO 13 J=1,NUMBER
007                POWER=I
008             13 P(I)=P(I)+X(J)**POWER
                C
                C
                C     DEVELOPING THE COEFFICIENTS AND THE CONSTANT TERMS OF THE NORMAL
                C     EQUATIONS.
                C
                C
009                N=M+1
010                DO 30 I=1,N
011                DO 30 J=1,N
012                K=I+J-2
013                IF(K)29,29,28
014             28 A(I,J)=P(K)
015                GO TO 30
016             29 A(1,1)=NUMBER
017             30 CONTINUE
018                B(1)=0.
019                DO 21 J=1,NUMBER
020             21 B(1)=B(1)+Y(J)
021                DO 22 I=2,N
022                B(I)=0.
023                DO 22 J=1,NUMBER
024             22 B(I)=B(I)+Y(J)*X(J)**(I-1)
                C
                C     PIVOTAL CONDENSATION
                C
025                NM1=N-1
026                DO 300 K=1,NM1
027                KP1=K+1
028                L=K
029                DO 400 I=KP1,N
030                IF(DABS(A(I,K))-DABS(A(L,K)))400,400,401
```

```
31            401 L=I
32            400 CONTINUE
33                IF(L-K)500,500,405
34            405 DO 410 J=K,N
35                TEMP=A(K,J)
36                A(K,J)=A(L,J)
37            410 A(L,J)=TEMP
38                TEMP=B(K)
39                B(K)=B(L)
40                B(L)=TEMP
              C
              C     ELIMINATION,BACK SOLUTION, AND PRINTING RESULTS
              C
41            500 DO 300 I=KP1,N
42                FACTOR=A(I,K)/A(K,K)
43                A(I,K)=0.0
44                DO 301 J=KP1,N
45            301 A(I,J)=A(I,J)-FACTOR*A(K,J)
46            300 B(I)=B(I)-FACTOR*B(K)
47                C(N)=B(N)/A(N,N)
48                I=NM1
49            710 IP1=I+1
50                SUM=0.0
51                DO 700 J= IP1,N
52            700 SUM=SUM+A(I,J)*C(J)
53                C(I)=(B(I)-SUM)/A(I,I)
54                I=I-1
55                IF(I)800,800,710
56            800 RETURN
57                END
```

APPENDIX D

TABULATED THERMODYNAMIC PROPERTIES

In this appendix values of free energy, enthalpy, heat capacity and entropy, as predicted by the polynomial coefficients listed in Appendix A, are given in tabular form. Each table contains, in addition to the above tabulations, the corresponding polynomial constants and the original source of the data from which the constants were evaluated.

POLYNOMIAL CONSTANTS AND THERMODYNAMIC PROPERTIES OF A+
OVER A TEMPERATURE RANGE OF 1000 TO 6000 DEGREES KELVIN.
REFERENCE TEMPERATURE = 298.16

T(K)	-(F-H*)/RT	(H-H*)/RT	S/R	CP/R	H/RT
1000	0.205521E 02	0.263107E 01	0.231832E 02	0.268569E 01	0.185476E 03
1200	0.210327E 02	0.264051E 01	0.236732E 02	0.268865E 01	0.155011E 03
1400	0.214403E 02	0.264723E 01	0.240875E 02	0.268557E 01	0.133251E 03
1600	0.217941E 02	0.265158E 01	0.244457E 02	0.267774E 01	0.116930E 03
1800	0.221065E 02	0.265388E 01	0.247604E 02	0.266631E 01	0.104234E 03
2000	0.223862E 02	0.265444E 01	0.250406E 02	0.265233E 01	0.940768E 02
2200	0.226392E 02	0.265355E 01	0.252927E 02	0.263677E 01	0.857648E 02
2400	0.228700E 02	0.265148E 01	0.255214E 02	0.262049E 01	0.788368E 02
2600	0.230821E 02	0.264847E 01	0.257306E 02	0.260424E 01	0.729734E 02
2800	0.232782E 02	0.264474E 01	0.259230E 02	0.258867E 01	0.679465E 02
3000	0.234606E 02	0.264052E 01	0.261011E 02	0.257436E 01	0.635888E 02
3200	0.236308E 02	0.263598E 01	0.262668E 02	0.256175E 01	0.597750E 02
3400	0.237905E 02	0.263129E 01	0.264218E 02	0.255120E 01	0.564092E 02
3600	0.239408E 02	0.262660E 01	0.265674E 02	0.254296E 01	0.534168E 02
3800	0.240827E 02	0.262204E 01	0.267047E 02	0.253719E 01	0.507391E 02
4000	0.242170E 02	0.261770E 01	0.268347E 02	0.253394E 01	0.483289E 02
6200	0.253581E 02	0.259561E 01	0.279537E 02	0.257947E 01	0.320867E 02
6400	0.254405E 02	0.259503E 01	0.280355E 02	0.257411E 01	0.311645E 02
4600	0.245821E 02	0.260685E 01	0.271889E 02	0.253836E 01	0.423557E 02
4800	0.246930E 02	0.260410E 01	0.272971E 02	0.254373E 01	0.406968E 02
5000	0.247992E 02	0.260182E 01	0.274011E 02	0.255038E 01	0.391708E 02
5200	0.249013E 02	0.259998E 01	0.275012E 02	0.255777E 01	0.377624E 02
5400	0.249993E 02	0.259856E 01	0.275979E 02	0.256525E 01	0.364587E 02
5600	0.250938E 02	0.259749E 01	0.276913E 02	0.257205E 01	0.352483E 02
5800	0.251850E 02	0.259671E 01	0.277817E 02	0.257735E 01	0.341217E 02
6000	0.252730E 02	0.259612E 01	0.278691E 02	0.258017E 01	0.330703E 02

A1	A2	A3	A4	A5	A6	A7
0.252945E 01	0.315090E-03	-0.196105E-06	0.398768E-10	-0.261838E-14	0.182845E 06	0.548071E 01

SOURCE OF DATA* W.G. BROWNE (ENGR PHYS TECH MEMO 2) APPENDIX A

REMAINDER OF APPENDIX D AVAILABLE ON REQUEST