A Technical Report

on

THERMODYNAMIC PROPERTIES IN POLYNOMIAL FORM

FOR CARBON, HYDROGEN, NITROGEN, AND

OXYGEN SYSTEMS FROM 300 TO 15000°K

by

D. D. Esch, Research Associate
A. Siripong, Research Assistant
R. W. Pike, Associate Professor
Co-Principal Investigator

NASA-RFL-TR-70-3

Prepared under Grant NGR19-001-059

for

Langley Research Center

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

November 15, 1970
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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 \( \text{H}_2, \text{N}_2, \text{O}_2, \text{Ne}, \text{Ar}, \text{He}, \text{C} \) (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

The authors would like to give acknowledgment to Dean Mayers and James Callender for their helpful assistance in collecting and analyzing the data. Special thanks is also given to Mrs. Sue Mayers for the typing of this report.
NOMENCLATURE

\( C_P^o \)  
heat capacity per mole at constant pressure

\( \Delta F_T^o \)  
standard free energy of a pure substance at temperature \( T \)

\( \Delta H_T^o \)  
standard enthalpy of a pure substance at temperature \( T \)

\( \Delta H_0^o \)  
standard enthalpy of a pure substance at a temperature of \( 0^oK \)

\( R \)  
universal gas constant, 1.987 cal/mole\(^oK\)

\( S_T^o \)  
standard entropy of a pure substance at temperature \( T \)

\( T \)  
absolute temperature

\( Y_i \)  
mole fraction of species \( i \)

\( (\Delta H_f^o)_T \)  
standard heat of formation at temperature \( T \)

Subscripts:

\( i \)  
refers to species

\( T \)  
absolute temperature (\(^oK\))

\( P \)  
constant pressure

Superscripts:

\( ^o \)  
denotes the standard state (pure substance at 1 atmosphere pressure)
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABSTRACT</td>
<td>ii</td>
</tr>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>iii</td>
</tr>
<tr>
<td>NOMENCLATURE</td>
<td>iv</td>
</tr>
<tr>
<td>I  INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>II  MATHEMATICAL DEVELOPMENT</td>
<td>2</td>
</tr>
<tr>
<td>III DISCUSSION OF RESULTS</td>
<td>8</td>
</tr>
<tr>
<td>IV SUMMARY</td>
<td>13</td>
</tr>
<tr>
<td>V  BIBLIOGRAPHY</td>
<td>15</td>
</tr>
<tr>
<td>APPENDIX A. Tabulated Constants for Polynomial Approximation</td>
<td>17</td>
</tr>
<tr>
<td>of Thermodynamic Properties</td>
<td></td>
</tr>
<tr>
<td>APPENDIX B. Determination of $(\Delta H_f^\circ)_298.16$ from $(\Delta H_f^\circ)_0$</td>
<td>29</td>
</tr>
<tr>
<td>APPENDIX C. Listing of Computer Data</td>
<td>33</td>
</tr>
<tr>
<td>APPENDIX D. Tabulated Thermodynamic Properties</td>
<td>40</td>
</tr>
<tr>
<td>VI DISTRIBUTION</td>
<td></td>
</tr>
</tbody>
</table>

V
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, \((H_T^o - H_0^o)/RT\) and \((F_T^o - H_0^o)/RT\) where the superscript \(o\) denotes the quantity at standard state (the pure component at 1 atmosphere pressure). The properties \(H_T^o\) and \(F_T^o\) 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:

\[
\begin{align*}
\text{d}H^o &= C_p^o \text{d}T \\
\text{d}S^o &= \frac{C_p^o \text{d}T}{T}
\end{align*}
\] (1)
Standard heat capacity data can be conveniently fitted to the following polynomial form:

\[ C_p^0 = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \] (3)

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

\[ S_T^0 = a_1 \ln T + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7 \] (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

\[ dF^0 = dH^0 - d(TS^0) = dH^0 - TdS^0 - S_T dT \] (5)

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

\[ dH^0 = TdS^0 \] (6)

therefore

\[ dF^0 = -S_T^0 dT \] (7)

Integrating this expression in temperature from absolute zero with \( S_T^0 \) defined by Equation (4) yields the following

\[ F_T^0 - F_0^0 = \left[ a_1 (\ln T - 1) + \frac{a_2 T^2}{2} + \frac{a_3 T^3}{6} + \frac{a_4 T^4}{12} + \frac{a_5 T^5}{20} + a_7 T \right] \] (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

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

(9)


From Equations (1) and (3) the comparable polynomial expression for standard enthalpy can be derived.

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

(10)

We have thus derived polynomial expressions for the thermodynamic functions of standard entropy, enthalpy and free energy relative to $0^\circ$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 $298^\circ$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, $H_0^\circ$. For an element, $H_0^\circ$ 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 $H_0^\circ$.

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

(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
\[
\frac{H^0}{RT} = \frac{(AH_f)_{Tref} - (H^0 - H^0)_{Tref}}{RT} \tag{12}
\]

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

\[
\frac{F^0}{RT} = A_1(1 - \ln T) - \frac{A_2}{2}T - \frac{A_3}{6}T^2 - \frac{A_4}{12}T^3 - \frac{A_5}{20}T^4 + \frac{A_6}{T} - A_7 \tag{13}
\]

\[
\frac{H^0}{RT} = A_1 + \frac{A_2}{2}T + \frac{A_3}{3}T^2 + \frac{A_4}{4}T^3 + \frac{A_5}{5}T^4 + \frac{A_6}{T} \tag{14}
\]

where \(A_6 = \frac{H^0}{R} = \left[\frac{(\Delta H_f)_{Tref} - (H^0 - H^0)_{Tref}}{R}\right] \)

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

\[
\frac{C_p^o}{R} = A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4
\]  
(A)

Enthalpy

\[
\frac{H_T^o}{RT} = A_1 + \frac{A_2}{2} T + \frac{A_3}{3} T^2 + \frac{A_4}{4} T^3 + \frac{A_5}{5} T^4 + \frac{A_6}{T}
\]  
(B)

Entropy

\[
\frac{S_T^o}{R} = A_1 \ln T + A_2 + \frac{A_3}{2} T^2 + \frac{A_4}{3} T^3 + \frac{A_5}{4} T^4 + A_7
\]  
(C)

Free Energy

\[
\frac{F_T^o}{RT} = A_1 (1-\ln T) - \frac{A_2}{2} T - \frac{A_3}{6} T^2 - \frac{A_4}{12} T^3 - \frac{A_5}{20} T^4 + \frac{A_6}{T} + A_7
\]  
(D)
\[
\frac{H^\circ_T - H^\circ_0}{RT} = B_1 + B_2 T + B_3 T^2 + B_4 T^3 + B_5 T^4
\]  \hspace{1cm} (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\(^\circ\)K and at 0\(^\circ\)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.

\[
A_7 = A_1 (1-\ln T) - \frac{A_2}{2} - \frac{A_3 T^2}{6} - \frac{A_4 T^4}{12} - \frac{A_5 T^5}{20} - \left( \frac{F^\circ_T - H^\circ_0}{RT} \right)
\]  \hspace{1cm} (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 were 1000-7000\(^\circ\)K and 5000-18000\(^\circ\)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\(^\circ\)K and 1000-6000\(^\circ\)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,

\[ C_p^\circ = \sum Y_i C_{p_i}^\circ + \sum H_i^\circ \left( \frac{\partial Y_i}{\partial T} \right) \] (18)

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

\( \text{IV. SUMMARY} \)

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.
V. BIBLIOGRAPHY


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.

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

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

\[
\frac{C_P}{R} = A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4
\]

\[
\frac{S_T}{R} = A_1 \ln T + A_2 T + \frac{A_3}{2} T^2 + \frac{A_4}{3} T^3 + \frac{A_5}{4} + A_7
\]

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

- **SPECIE**
  - pure component

- **CODE**
  - 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
| CH   | C.3545E 01 | 0.3795E-04 | -0.1826E-05 | 0.4455E-08 | -0.2186E-11 | 0.7060E 05 | 0.1824E 01 | *M1   |
|      | C.3183E 01 | 0.8461E-03 | -0.2442E-06 | 0.3107E-10 | -0.1353E-14 | 0.7061E 05 | 0.3504E 01 | B2    |
|      | C.3906E 01 | 0.1127E-03 | 0.2193E-07  | -0.1693E-11| 0.2844E-16  | 0.7061E 05 | -0.6141E 00| B3    |
| CH2  | C.3531E 01 | -0.2507E-02 | 0.1235E-04  | -0.1175E-07| 0.3812E-11  | 0.3365E 05 | 0.1797E 01 | *M1   |
|      | C.3274E 01 | 0.2638E-02  | -0.7538E-06 | 0.9695E-10 | -0.4625E-14 | 0.3365E 05 | 0.3183E 01 | B2    |
|      | C.4553E 01 | 0.9757E-03  | -0.1478E-06 | 0.9828E-11 | -0.2402E-15 | 0.3365E 05 | -0.4053E 01| B3    |
| CH3  | C.3408E 01 | 0.4268E-02  | 0.2033E-06  | -0.1155E-08| 0.4129E-12  | 0.1565E 05 | 0.2704E 01 | *M1   |
|      | C.3528E 01 | 0.5212E-02  | -0.1680E-05 | 0.2399E-09 | -0.1251E-13 | 0.1472E 05 | 0.1893E 01 | B2    |
|      | C.6151E 01 | 0.1553E-02  | -0.2364E-06 | 0.1576E-10 | -0.3859E-15 | 0.1472E 05 | -0.1272E 02| B3    |
| CH4  | C.4259E 01 | -0.6913E-07 | 0.3166E-04  | -0.2971E-07| 0.9510E-11  | -0.1019E 05| 0.9175E 00 | *M1   |
|      | C.2234E 01 | 0.8929E-02  | -0.2946E-06 | 0.4264E-09 | -0.2238E-13 | 0.1021E 05 | 0.6764E 01 | B2    |
|      | C.601E 01  | 0.2665E-02  | -0.4192E-06 | 0.2888E-10 | -0.7251E-15 | 0.1021E 05 | -0.1751E 02| B3    |
| CN   | C.3353E 01 | 0.2763E-02  | 0.6357E-05  | -0.5413E-08| 0.1451E-11  | 0.4741E 05 | 0.2972E 01 | *M1   |
|      | C.3411E 01 | 0.4579E-03  | 0.1005E-06  | 0.3573E-10 | 0.2361E-14  | 0.4745E 05 | 0.4746E 01 | B2    |
|      | C.3478E 01 | 0.7337E-03  | -0.9088E-07 | 0.4847E-11 | -0.1018E-15 | 0.5420E 05 | 0.4152E 01 | B3    |
| CO+  | C.3144E 01 | 0.1265E-02  | -0.4715E-06 | 0.7965E-10 | -0.4421E-14 | 0.1490E 06 | 0.6051E 01 | B3    |
|      | C.4076E 01 | 0.1498E-03  | 0.1644E-06  | 0.9201E-11 | -0.2310E-15 | 0.1490E 06 | 0.9992E 00 | B3    |
| CO   | C.3787E 01 | -0.2171E-02 | 0.5670E-05  | -0.3474E-08| 0.7722E-12  | -0.1436E 05| 0.2634E 01 | *M1   |
|      | C.3254E 01 | 0.9469E-03  | -0.2047E-06 | 0.3037E-10 | -0.1177E-14 | 0.4875E 01 | 0.4875E 01 | B2    |
|      | C.3366E 01 | 0.1027E-03  | -0.1968E-06 | 0.1940E-10 | -0.5949E-15 | 0.1434E 05 | 0.4263E 01 | B3    |
| CO2  | C.2173E 01 | 0.1038E-01  | -0.1673E-04 | 0.6345E-03 | -0.1620E-11 | -0.4835E 05| 0.1066E 02 | *M1   |
|      | C.4413E 01 | 0.3192E-02  | -0.1298E-05 | 0.2415E-09 | -0.1674E-13 | -0.4894E 05| 0.7288E 00 | *M2   |

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|      |    |    |    |    |    |    |    |    |    |    |    |    | 0.2727E 01 | 0.142 CE-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 | 0.6453E-02 | -0.2299E-05 | 0.3739E-09 | -0.2461E-13 | -0.6401E 04 | 0.982CE 05 | *M2 |
| NO+  |    |    |    |    |    |    |    |    |    |    |    |    | 0.328CE 01 | 0.1929E-02 | -0.3075E-06 | 0.4028E-10 | -0.1814E-14 | 0.1184E 06 | 0.5225E 01 | E2  |
|      |    |    |    |    |    |    |    |    |    |    |    |    | 0.3561E 01 | 0.6026E-03 | -0.1546E-06 | 0.1697E-10 | -0.5296E-15 | 0.1184E 06 | 0.3176E 01 | E3  |
| 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 | 0.6910E 01 | *E2  |
|      |    |    |    |    |    |    |    |    |    |    |    |    | 0.3345E 01 | 0.2521E-03 | -0.2658E-07 | 0.2162E-11 | -0.6381E-16 | 0.9764E 04 | 0.3212E 01 | E3  |
| 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 | 0.263E-02 | -0.1095E-05 | 0.2082E-09 | -0.1465E-13 | 0.234E 04 | 0.1368E 01 | *M2 |
| NS   |    |    |    |    |    |    |    |    |    |    |    |    | 0.4562E 01 | -0.2819E-02 | 0.9316E-05 | -0.959E-08 | 0.3284E-11 | 0.3087E 05 | 0.4081E 01 | *M1 |
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| N2+  |    |    |    |    |    |    |    |    |    |    |    |    | 0.3397E 01 | 0.4525E-03 | 0.1272E-06 | -0.3879E-10 | 0.2459E-14 | 0.1626E 06 | 0.4205E 01 | E2  |
|      |    |    |    |    |    |    |    |    |    |    |    |    | 0.337CE 01 | 0.8629E-03 | -0.1476E-06 | 0.8037E-11 | -0.1940E-15 | 0.1826E 06 | 0.4073E 01 | E3  |
| N2   |    |    |    |    |    |    |    |    |    |    |    |    | 0.3592E 01 | -0.1333E-02 | 0.2650E-05 | -0.9769E-09 | 0.9977E-13 | 0.1063E 04 | 0.2287E 01 | *M1 |
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|      |    |    |    |    |    |    |    |    |    |    |    |    | 0.3727E 01 | 0.4684E-03 | -0.1146E-06 | 0.1154E-10 | -0.3293E-15 | -0.1043E 04 | 0.1294E 01 | E3  |
| 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 |    |    |    |    |    |    |    |    |    |    |    |    | 0.3155E 01 | 0.2719E-01 | -0.2535E-04 | 0.1099E-07 | 0.1660E-11 | 0.7673E 03 | 0.1148E 02 | *M1 |
|      |    |    |    |    |    |    |    |    |    |    |    |    | 0.1643E 01 | 0.6036E-02 | -0.2583E-05 | 0.4928E-09 | 0.3478E-13 | -0.2741E 04 | 0.2582E 02 | *M2 |</p>
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<th>Column 4</th>
<th>Column 5</th>
<th>Column 6</th>
<th>Column 7</th>
<th>Column 8</th>
<th>Column 9</th>
<th>Column 10</th>
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<td>-0.3726E-06</td>
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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,

\[ (\Delta H_f^0)_{298.16} = (\Delta H_f^0)_0 + \Delta H_1 + \Delta H_2 \]  \hspace{1cm} (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; H₂, N₂, O₂, 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>
<thead>
<tr>
<th>Component</th>
<th>Reaction</th>
<th>(AH\textsubscript{f})\textsuperscript{298.16} (Kcal/gmole)</th>
<th>(AH\textsubscript{f})\textsuperscript{0} (Kcal/gmole)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>1/2 N\textsubscript{2} → N</td>
<td>112.951</td>
<td>112.507</td>
<td>2</td>
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<tr>
<td>O</td>
<td>1/2 O\textsubscript{2} → O</td>
<td>59.544</td>
<td>58.972</td>
<td>2</td>
</tr>
<tr>
<td>C (gas)</td>
<td>C → C</td>
<td>171.301</td>
<td>169.990</td>
<td>2</td>
</tr>
<tr>
<td>A\textsuperscript{+}</td>
<td>A → A\textsuperscript{+} + e\textsuperscript{-}</td>
<td>364.828</td>
<td>363.345</td>
<td>2</td>
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<tr>
<td>N\textsuperscript{+}</td>
<td>1/2 N\textsubscript{2} → N\textsuperscript{+} + e\textsuperscript{-}</td>
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<td>447.564</td>
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<tr>
<td>O\textsuperscript{+}</td>
<td>1/2 O\textsubscript{2} → O\textsuperscript{+} + e\textsuperscript{-}</td>
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<td>372.942</td>
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<td>C\textsubscript{s} → C\textsuperscript{+} + e\textsuperscript{-}</td>
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<td>429.537</td>
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<td>497.186</td>
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<td>C\textsubscript{s} → C\textsuperscript{++} + 2e\textsuperscript{-}</td>
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<td>991.689</td>
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<td>$(\Delta H_f^0)_0$ (Kcal/gmole)</td>
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</tr>
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<td>74.1277</td>
<td>73.400</td>
<td>4</td>
</tr>
<tr>
<td>C$^3$</td>
<td>$3C_s \rightarrow C_3$</td>
<td>189.6115</td>
<td>188.000</td>
<td>4</td>
</tr>
<tr>
<td>C$^-$</td>
<td>$C_s + e^- \rightarrow C^-$</td>
<td>142.2300</td>
<td>141.000</td>
<td>4</td>
</tr>
</tbody>
</table>
APPENDIX C

LISTING OF COMPUTER PROGRAM
**PROGRAM FOR CURVE-FIT OF THERMODYNAMIC FUNCTIONS**

This program calculates the values of the constants A1-A7 for the polynomial forms of the free energy, enthalpy, heat capacity, and entropy relationships as used in McBride, et al., NASA SP-3001, pp. 14-15.

The following input data are required:

1. **Identification Card** -- Consists of species name in cols. 1-8, reference temperature in cols. 16-22, delta H of formation at the reference temperature (cal/mole) in cols. 32-46, and the value of the enthalpy function at the reference temperature (cal/mole) in cols. 51-60. All numerical entries on this card are to be in F-format.

2. **Source Card** -- Cols. 1-79 are available for a brief bibliographical citation.

3. **Function Data Cards** -- These cards contain temperatures in cols. 1-6, and the corresponding values of the free energy and enthalpy functions respectively in cols. 7-20 and 21-34. The form of these functions as required for input can be varied. In general, tabulated data is of the form of \(-(F-H*)/T\). If the data is of the form of \(-(F-H*)\), the number 1 can be inserted in col. 80 of the source card and the input will be transformed internally to the general form.

4. **Termination Card** -- A negative value in cols. 1-6 will terminate data input. After this package has been processed a new set of cards will be read.

---

Donald D. Esch
Louisiana State University
August 1973

**001**
**002**
**003**
**004**
**005**
**006**
**007**
**008**
**009**
**010**
**011**
**012**
**013**
**014**
**015**

**Double Precision** T(100), H(100), B(7)
**Dimension** SOURCE(39), SP(2), F(100), HC(100), FC(100), A(7)
**Dimension** S(100), CP(100), HH(100)
**Integer Range**
**R=1.98718**
**I=1**
**READ 100, SP, TRER, DELH, HREF**
**READ 101, SOURCE, NTYPE**
**READ 102, T(I), F(I), H(I)**
**IF(T(I),LT,G.0)GOTO30**
**I=I+1**
**GOTO20**
**NUMBER=I-1**
**TREF=298.16**

**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**

**C** SET UP ARRAYS FOR LEAST SQUARES FIT.
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**
**C**

**DO501=1, NUMBER**
35

ITRAN IV G LEVEL 18

MAIN

DATE = 71062 18/05/4

016  H(I) = H(I)/R
017  F(I) = =F(I)/R
018  IF(NTYPE.EQ.0)GOTO70
019  DO60 I=1,NUMBER
020  H(I) = H(I)/T(I)
021  60  F(I) = F(I)/T(I)
022  70  CONTINUE

C

C CALL LSFIT(T,H,NUMBER,4,B)

C

A(1) = B(1)
A(2) = B(2)*2.
A(3) = B(3)*3.
A(4) = B(4)*4.
A(5) = B(5)*5.

C-----DETERMINE THE VALUE OF A(6)

C

HZERO = DELH - HREF
A(6) = HZERO/R

C-----Determine the value of A(7)

C

SUMA7 = 0.0
DO80 I = 1, NUMBER
TEMP = T(I)
FEST = A(1)*(1 - ALOG(TMP)) - A(2)*T(I)/2. - A(3)*T(I)*2)/6. - A(4)*
1 (T(I))**3)/12. - A(5)*T(I)*4)/20.
DF = FEST - F(I)
SUMA7 = SUMA7 + DF
A(7) = SUMA7/NUMBER

C-----Determine Temperature Range--Range 1 include temperatures from

C 3 TO 1300, Range 2 from 1000 TO 6000, and Range 3 from 6000 TO

C 18000 DEGREES KELVIN.

C

RANGE = 1
IF(NUMBER .LE. 1000) GOTO85
RANGE = 2
IF(T(NUMBER) .LE. 8000) GOTO85
RANGE = 3
CONTINUE

C-----Output

C-----Punch out thermo data cards for CHEMSEQ program

DO88 N = 1, 20
WRITE(7,117)(A(I), I=1,7), SP, RANGE

PRINT 113
PRINT 103, SP
IF (RANGE .LT. 3) GOTO47
IF(T(NUMBER).EQ.1000) GO TO 51
ITLO = 6000
ITHI = 15000
JANE = 6
JIM = 24
GO TO 49

ITLO=6000

ITHI=10000

JANE=6

JIM=26

GOTO49

ITLO=1000

ITHI=6000

JANE=1

JIM=26

PRINT 104, ITLO, ITHI

PRINT 105, TREF

PRINT 108

DO901=JANF, JIM

TEMP=T(I)


A(5)*(T(I)**4)/5.*A(6)/T(I)


A(5)*(T(I)**4)/5.*A(7)

CP(I)=A(1) + A(2)*T(I) + A(3)*T(I)**2 + A(4)*T(I)**3 +

A(5)*(T(I)**4)

S(I)=A(6)/A(7)

HTO=HC(I) + A(6)/T(I)

NT=T(I)

PRINT 112, NT, FC(I), HC(I), S(I), CP(I), HTO

PRINT 108

PRINT 109

PRINT 110,(A(I), I=1,7)

PRINT 111, SOURCE

NN=JIM-JANE

NCOUNT=26-NN

IF(NCOUNT.LT.1)NCOUNT=1

DO95N=1, NCOUNT

PRINT 116

PRINT 114

WRITE(6,117)(A(I), I=1,7), SP, RANGE

PRINT 115

GOTO10

STOP

C

C---- FORMAT STATEMENTS

C

100 FORMAT(2A3,9X,F6.2,T10X,F14.5,F5X,F10.2)

101 FORMAT(39A2,12)

102 FORMAT(F6.0,2E14.4)

103 FORMAT(25X,'POLYNOMIAL CONSTANTS AND THERMODYNAMIC PROPERTIES OF ' 1,2A3)

104 FORMAT(25X,'OVER A TEMPERATURE RANGE OF ',T15,' TO ',T15,' DEGREES K ' 1ELVIN. ')

105 FORMAT(37X,'REFERENCE TEMPERATURE = ',F6.2,'/1)

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**  
18/05/45

```fortran
098 108 FORMAT(10X,18('-----'),/)  
109 FORMAT(  
16X,'A01',11X,'A02',11X,'A03',11X,'A04',11X,'A05',  
11X,'A06',11X,'A07')  
110 FORMAT(10X,7(E13.6),/)  
111 FORMAT(8X,'SOURCE OF DATA',5X,3A2)  
112 FORMAT(10X,18,5E16.6)  
113 FORMAT(1H1,/,22('-----'),7(/,' ',108X,' '))  
114 FORMAT(  
22('-----'))  
115 FORMAT(1H1)  
116 FORMAT(' ',108X,' ')  
117 FORMAT(7E10.4,2X,2A3,1X,11)  
118 FORMAT(F20.2)  
119 END
```
SUBROUTINE LSFIT(X,Y,NUMBER,M,C)

LEAST SQUARE CURVE FITTING OF ANY ORDER POLYNOMIAL
OF ORDER EQUAL TO OR LESS THAN 10

NUMBER IS THE ACTUAL NUMBER OF X-Y DATA PAIRS. MAXIMUM OF 200
M IS THE DEGREE OF THE POLYNOMIAL MAXIMUM OF 10
N IS THE NUMBER OF EQUATIONS (=M+1)
X,Y IS THE ARRAY FOR THE DATA PAIRS
A IS THE ARRAY FOR THE SUM, WHICH BECOME THE COEFFICIENTS OF THE
UNKNOWN IN THE SIMULTANEOUS EQUATIONS.
B IS THE ARRAY FOR THE CONSTANT TERMS IN THE SIMULTANEOUS EQUATIONS
C IS THE ARRAY FOR THE UnknownS, WHICH BECOME THE COEFFICIENTS IN
THE POLYNOMIAL.
P IS THE ARRAY FOR THE POWERS OF THE X(I), FROM 1 TO 2M.

REAL*8
X(100), Y(100), A(7, 7), B(7), C(7), P(20)

MX2=M*2
DO 13 I=1, MX2
P(I)=C*0
DO 13 J=1, NUMBER
POWER=I
13 P(I)=P(I)*X(J)**POWER

DEVELOPING THE COEFFICIENTS AND THE CONSTANT TERMS OF THE NORMAL
EQUATIONS.

N=M+1
DO 30 I=1, N
DO 30 J=1, N
K=I+J-2
IF(K)29, 29, 28
28 A(I, J)=P(K)
GO TO 30
29 A(I, 1)=NUMBER
30 CONTINUE
B(1)=0.
DO 21 J=1, NUMBER
21 B(1)=B(1)+Y(J)
DO 22 I=2, N
B(I)=C.
DO 22 J=1, NUMBER
22 B(I)=B(I)+Y(J)*X(J)**(I-1)

PIVOTAL CONDENSATION

NM1=N-1
DO 300 K=1, NM1
KP1=K+1
L=K
DO 400 I=KP1, N
IF(DABS(A(I, K))-DABS(A(L, K)))400,40C, 401

300 CONTINUE
TRAN IV G LEVEL 18

LSFIT

DATE = 71062
18/05/46

31  401 L=1
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

41  500 DO 300 I=KP1,N
42      FACTOR=A(I,K)/A(K,K)
43      A(I,K)=0.0
44  300 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)=C(N)/A(N,N)
48  I=NM1
49  710 IP1=I+1
50      SUM=0.0
51  700 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  700 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

<table>
<thead>
<tr>
<th>T(K)</th>
<th>-(F-H*)/RT</th>
<th>(H-H*)/RT</th>
<th>S/R</th>
<th>CP/R</th>
<th>H/RT</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>0.205521E 02</td>
<td>0.263107E 01</td>
<td>0.231832E 02</td>
<td>0.268569E 01</td>
<td>0.185476E 03</td>
</tr>
<tr>
<td>1200</td>
<td>0.210327E 02</td>
<td>0.264051E 01</td>
<td>0.236732E 02</td>
<td>0.268865E 01</td>
<td>0.155011E 03</td>
</tr>
<tr>
<td>1400</td>
<td>0.214403E 02</td>
<td>0.264723E 01</td>
<td>0.240875E 02</td>
<td>0.268557E 01</td>
<td>0.133251E 03</td>
</tr>
<tr>
<td>1600</td>
<td>0.217941E 02</td>
<td>0.265158E 01</td>
<td>0.244457E 02</td>
<td>0.267774E 01</td>
<td>0.116930E 03</td>
</tr>
<tr>
<td>1800</td>
<td>0.221065E 02</td>
<td>0.265388E 01</td>
<td>0.247604E 02</td>
<td>0.266631E 01</td>
<td>0.104234E 03</td>
</tr>
<tr>
<td>2000</td>
<td>0.223862E 02</td>
<td>0.265444E 01</td>
<td>0.250406E 02</td>
<td>0.265233E 01</td>
<td>0.940768E 02</td>
</tr>
<tr>
<td>2200</td>
<td>0.226392E 02</td>
<td>0.265355E 01</td>
<td>0.252927E 02</td>
<td>0.263677E 01</td>
<td>0.857648E 02</td>
</tr>
<tr>
<td>2400</td>
<td>0.228700E 02</td>
<td>0.265148E 01</td>
<td>0.255214E 02</td>
<td>0.262049E 01</td>
<td>0.788368E 02</td>
</tr>
<tr>
<td>2600</td>
<td>0.230821E 02</td>
<td>0.264847E 01</td>
<td>0.257306E 02</td>
<td>0.260424E 01</td>
<td>0.729734E 02</td>
</tr>
<tr>
<td>2800</td>
<td>0.232782E 02</td>
<td>0.264474E 01</td>
<td>0.259230E 02</td>
<td>0.258867E 01</td>
<td>0.679465E 02</td>
</tr>
<tr>
<td>3000</td>
<td>0.234606E 02</td>
<td>0.264052E 01</td>
<td>0.261011E 02</td>
<td>0.257436E 01</td>
<td>0.635888E 02</td>
</tr>
<tr>
<td>3200</td>
<td>0.236308E 02</td>
<td>0.263598E 01</td>
<td>0.262688E 02</td>
<td>0.256175E 01</td>
<td>0.597750E 02</td>
</tr>
<tr>
<td>3400</td>
<td>0.237905E 02</td>
<td>0.263129E 01</td>
<td>0.264218E 02</td>
<td>0.255120E 01</td>
<td>0.564092E 02</td>
</tr>
<tr>
<td>3600</td>
<td>0.239408E 02</td>
<td>0.262660E 01</td>
<td>0.265674E 02</td>
<td>0.254296E 01</td>
<td>0.534168E 02</td>
</tr>
<tr>
<td>3800</td>
<td>0.240827E 02</td>
<td>0.262204E 01</td>
<td>0.267047E 02</td>
<td>0.253719E 01</td>
<td>0.507391E 02</td>
</tr>
<tr>
<td>4000</td>
<td>0.242170E 02</td>
<td>0.261770E 01</td>
<td>0.268347E 02</td>
<td>0.253394E 01</td>
<td>0.483289E 02</td>
</tr>
<tr>
<td>4200</td>
<td>0.243419E 02</td>
<td>0.259561E 01</td>
<td>0.279537E 02</td>
<td>0.257947E 01</td>
<td>0.302867E 02</td>
</tr>
<tr>
<td>4400</td>
<td>0.244049E 02</td>
<td>0.259503E 01</td>
<td>0.280355E 02</td>
<td>0.257411E 01</td>
<td>0.311645E 02</td>
</tr>
<tr>
<td>4600</td>
<td>0.245821E 02</td>
<td>0.260685E 01</td>
<td>0.271889E 02</td>
<td>0.253836E 01</td>
<td>0.423557E 02</td>
</tr>
<tr>
<td>4800</td>
<td>0.246930E 02</td>
<td>0.260410E 01</td>
<td>0.272971E 02</td>
<td>0.254373E 01</td>
<td>0.406969E 02</td>
</tr>
<tr>
<td>5000</td>
<td>0.247992E 02</td>
<td>0.260182E 01</td>
<td>0.274011E 02</td>
<td>0.255036E 01</td>
<td>0.391708E 02</td>
</tr>
<tr>
<td>5200</td>
<td>0.249133E 02</td>
<td>0.259998E 01</td>
<td>0.275012E 02</td>
<td>0.255777E 01</td>
<td>0.377624E 02</td>
</tr>
<tr>
<td>5400</td>
<td>0.249993E 02</td>
<td>0.259856E 01</td>
<td>0.275979E 02</td>
<td>0.256525E 01</td>
<td>0.364587E 02</td>
</tr>
<tr>
<td>5600</td>
<td>0.250938E 02</td>
<td>0.259749E 01</td>
<td>0.276913E 02</td>
<td>0.257205E 01</td>
<td>0.352483E 02</td>
</tr>
<tr>
<td>5800</td>
<td>0.251850E 02</td>
<td>0.259671E 01</td>
<td>0.277817E 02</td>
<td>0.257735E 01</td>
<td>0.341217E 02</td>
</tr>
<tr>
<td>6000</td>
<td>0.252730E 02</td>
<td>0.259612E 01</td>
<td>0.278691E 02</td>
<td>0.258017E 01</td>
<td>0.330703E 02</td>
</tr>
</tbody>
</table>

A1 = 0.252945E 01 A2 = 0.315090E-03 A3 = 0.196105E-06 A4 = 0.398768E-10 A5 = 0.261838E-14 A6 = 0.192845E 06 A7 = 0.548071E 01

SOURCE OF DATA* W.G. BROWNE (ENGR PHYS TECH MEMO 2) APPENDIX A
REMAINDER OF APPENDIX D AVAILABLE ON REQUEST