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Technical Report 32-1350

A Program for Computing Shock-Tube Gasdynamic Properties

T. E. Horton
W. A. Menard

JET PROPULSION LABORATORY
CALIFORNIA INSTITUTE OF TECHNOLOGY
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Preface

The work described in this report was performed by the Environmental Sciences Division of the Jet Propulsion Laboratory (JPL).

One of the authors, T. E. Horton, is currently on the staff of the University of Mississippi.

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Abstract

A computer program for calculating the chemical equilibrium properties associated with moving, standing, and reflected normal shocks has been developed. The program calculates thermodynamic properties and chemical composition from basic spectroscopic data. Both dissociation and ionization over an unlimited temperature range can be considered. The chemical equilibrium and composition equations are developed from statistical mechanics, and the procedure for solving the coupled equilibrium and normal shock equations is presented. Flow diagrams, operating instructions, and listings of the program and input data are included. The program can treat initial mixtures consisting of up to ten gases. In this report, input data are listed for sixty-six species which are composed of carbon, nitrogen, oxygen, hydrogen, argon, neon, and helium.

A Program for Computing Shock-Tube Gasdynamic Properties

I. Introduction

Investigations of atomic and molecular phenomena utilizing shock tubes as well as studies of the feasibility of planetary entry at high velocities have created a need for rapid solution techniques for aerothermochemistry problems involving the high-temperature properties of gas mixtures. Although most problems in the field of aerothermodynamics are characterized by large force, chemical composition, and temperature gradients and thus by nonequilibrium phenomena, there are many processes of interest in this field for which either the gradients disappear or the reaction rates are sufficiently fast so that the assumption of chemical equilibrium is rational. This report, as in an earlier publication (Ref. 1), is confined to the problem of supplying thermodynamic properties and chemical composition of multi-component, high-temperature, real-gas mixtures which satisfy the conditions of chemical equilibrium.

The subject of equilibrium properties of dissociated and ionized gases is of interest in a variety of fields ranging from astrophysics to re-entry system design, and has been an active area of research as witnessed by the literature (Refs. 2–37). A review of this material is given in Appendix A. These published works can be categorized as those dealing primarily with (1) the physics of the subject, (2) the computational or formulational aspects of the subject, and (3) the presentation of computed property data. Work in the third category can be further divided into those in which long range interactions between particles are either neglected or included in some manner. Some authors term the former ideal or perfect real-gas mixtures and the latter as non-ideal or imperfect real-gas mixtures.

A variety of gases have been treated. However, data are usually presented in the form of a Mollier chart or tabulation with composition data presented only for a limited number of pressure or density levels. When this information is used to reduce data taken in a shock-tube experiment, the resulting uncertainty and effort are undesirable. The JPL Thermochemistry and Normal-Shock Computer Program was originally designed to alleviate this difficulty by completely mechanizing the process of generating parameters for moving, standing, and reflected shock conditions as experienced in shock tubes. As a result of this ability to handle a variety of possible gas-mixture combinations, the program has been used extensively by the staff at JPL.

However, because of the method used in handling the species' thermochemistry data, the temperature range was limited. Also, because the computations could be made only at temperatures for which library data were available, the determination of standing bow shock and reflected shock gas compositions was not possible except by plotting Mollier data computed for neighboring temperatures.

To eliminate these difficulties, a revised program has been written, one in which our goal was to retain the versatility and reliability of the old program, but in which the species' thermochemistry data, i.e., specific enthalpy and free energy, are generated internally from spectroscopic data. The generation of the specific enthalpy and free energy was to be handled by a subroutine so that the model used in computing these could be changed. The subroutine and problems associated with the computation of the partition function and thermochemistry data are discussed in Ref. 38. Also, the output format was to be handled through a subroutine which could be modified with ease.

The result of this revision is the present program which is written in Fortran II for use on an IBM 7090 or 7094 computer. The program calculates chemical equilibrium composition and the parameters associated with traveling, standing, and reflected normal shocks. The initial gas mixture, temperature, and pressure can be varied with ease. The program can treat initial mixtures consisting of up to ten gases. Both dissociation and ionization over an unlimited temperature range can be considered. The computational capacity of the program is a mixture of 100 different species composed of 10 different elements. These numbers are limited only by the initial dimension statement and can be increased, providing computer storage is available. The output is a complete thermodynamic and chemical description of the gas which satisfies the Hugoniot equation for the important normal shock cases which are useful in both shock-tube experimentation and free-flight entry calculations.

The program can also be used to generate Mollier thermodynamic data at selected temperatures and densities if this option is desired. A mathematical statement of the criterion for chemical equilibrium is given prior to further discussion of the details of the computer program.

II. Chemical Equilibrium

In an earlier report (Ref. 1), the mass action and mass balance equations, which yield the chemical composition for chemical equilibrium, were developed within the context of classical thermodynamics as in (Refs. 39, 40, and 41). In this section these same equations are developed with statistical mechanical arguments. The equations are then compared to the classical expressions to show the well known relationship between equilibrium constant, free energy, and partition function.

The problem is one of determining the most probable stationary distribution of atoms and electrons among the energy levels of chemical components of the mixture, subject to the constraint that the total mass of each element specie remain constant. Thus, for a mixture composed of m number of elemental species which combine to form s number of compounds, the compounds will be identified by the numbers $1, 2, \cdots, s$ and the elements by the numbers $s+1$, $s+2$, $s+3$, $\cdots, s+m$. Further, let the symbols $X^{(s+1)}$, $X^{(s+2)}$, $X^{(s+3)}$, $\cdots, X^{(s+m)}$ be used to represent the usual symbols for the chemical elements so that the compounds and ions of the mixture can be written as

$$Y^{(p)} = X_{\alpha_{p,\,s+1}}^{(s+1)} X_{\alpha_{p,\,s+2}}^{(s+2)} X_{\alpha_{p,\,s+3}}^{(s+3)} \cdots X_{\alpha_{p,\,s+m}}^{(s+m)}$$

where $p = 1, 2, 3, \cdots, s$. The α_{ij} indicates the number of atoms of the jth numbered element in the ith numbered specie. The α_{ij}'s come from the set of positive and negative real integers which include zero. The array of $(\alpha_{p,\,s+1}, \alpha_{p,\,s+2}, \alpha_{p,\,s+3}, \cdots, \alpha_{p,\,s+m})$ which represents the essentials of the chemical formula for the pth compound is termed the formula vector for the pth specie. The introduction of this concept by Brinkley (Refs. 42, 43, and 44) allows one to use the theory of linear vector space to formulate problems in stoichiometry.

To determine the arrangement of elementary specie among the $(s+m)$ different chemical combinations and the distribution of the chemical combinations among their q_k number of energy levels $\epsilon_1^{(k)}, \epsilon_2^{(k)}, \epsilon_3^{(k)}, \cdots, \epsilon_{q_k}^{(k)}$, each energy level having degeneracy $g_1^{(k)}, g_2^{(k)}, g_3^{(k)} \cdots, g_{q_k}^{(k)}$, respectively, one must find an array of occupation numbers or concentrations $N_1^{(k)}$, $N_2^{(k)}$, $N_3^{(k)}$, $\cdots, N_{q_k}^{(k)}$ for $k = 1, 2, 3, \cdots, s+m$, which represents their most probable arrangement. The most probable arrangement is the one that can be achieved in the greatest number of ways. If the assumptions are made that the long-range interactions between particles of the mixture are negligible so that the collision times are small compared to times between collisions and that the particles of a particular chemical specie are indistinguishable from each other, then from the theory of combinatory analysis we have the

number of ways $W_i^{(k)}$ in which $N_i^{(k)}$ objects can be distributed in $g_i^{(k)}$ distinguishable categories when there is no restriction on the number in each category given by

$$W_i^{(k)} = \frac{(g_i^{(k)})(g_i^{(k)}+1)(g_i^{(k)}+2)\cdots(g_i^{(k)}+N_i^{(k)}-1)}{N_i^{(k)}!} \tag{1}$$

For the usual chemical system, $g_i^{(k)} >> N_i^{(k)}$; so

$$W_i^{(k)} = \frac{(g_i^{(k)})^{N_i^{(k)}}}{N_i^{(k)}!} \tag{2}$$

Thus, for each specie the number of arrangements of its $N^{(k)}$ particle with $N_1^{(k)}, N_2^{(k)}, N_3^{(k)}, \cdots, N_{q_k}^{(k)}$ in each energy level is

$$W^{(k)} = \prod_{i=1}^{q_k} \frac{(g_i^{(k)})^{N_i^{(k)}}}{(N_i^{(k)})!} \tag{3}$$

And the number of arrangements for the mixture is

$$W = \prod_{k=1}^{s+m} W^{(k)} \tag{4}$$

The natural logarithm of the above expression can be written as

$$\ln W = \sum_{k=1}^{s+m}\sum_{i=1}^{q_k} N_i^{(k)}\left(\ln\frac{g_i^{(k)}}{N_i^{(k)}} + 1\right) \tag{5}$$

with the aid of Stirling's approximation, i.e.,

$$\ln N! = N(\ln N - 1)$$

for $N >> 1$. For the most probable arrangement, the above expression must be an extremium for variations in the $N_i^{(k)}$'s subject to the constraints ① that the total number or mass of elemental species is a constant, i.e.,

$$\sum_{j=1}^{q_e} dN_j^{(e)} + \sum_{k=1}^{s}\sum_{i=1}^{q_k} \alpha_{ke}\, dN_i^{(k)} = 0 \tag{6}$$

for $e = s+1, s+2, s+3, \cdots, s+m$ and ② that the total energy of the system remain constant, i.e.,

$$\sum_{k=1}^{s+m}\sum_{i=1}^{q_k} \epsilon_i^{(k)}\, dN_i^{(k)} = 0 \tag{7}$$

(Note that the above expression assumes that the energies of the individual states are independent of variations in the concentrations. This is valid only when the long-range interactions are negligible.) For W to have an extreme value, the differential of Eq. (5) must be zero; so

$$\sum_{k=1}^{s+m}\sum_{i=1}^{q_k} \ln\frac{g_i^{(k)}}{N_i^{(k)}}\, dN_i^{(k)} = 0 \tag{8}$$

Now using the technique of Legrangian multipliers, we find from the combination of Eqs. (7) and (8) with the m equations of the type of Eq. (6) that

$$N_i^{(k)} = g_i^{(k)} \prod_{e=s+1}^{s+m} (\exp\gamma_e)^{\alpha_{ke}} (\exp\beta\epsilon_i^{(k)}) \tag{9}$$

for $i = 1, 2, 3, \cdots, q_k$ and $k = 1, 2, 3, \cdots, s$ and that

$$N_j^{(e)} = g_j^{(e)} \exp(\gamma_e) \exp(\beta\epsilon_j^{(e)}) \tag{10}$$

for $j = 1, 2, 3, \cdots, q_e$ and $e = s+1, s+2, \cdots, s+m$. Summing the above expressions over all energy states gives

$$N^{(k)} = \sum_{i=1}^{q_k} N_i^{(k)} = \prod_{e=s+1}^{s+m} (\exp\gamma_e)^{\alpha_{ke}} \sum_{i=1}^{q_k} g_i^{(k)} \exp(\beta\epsilon_i^{(k)}) \tag{11}$$

for $k = 1, 2, 3, \cdots, s$ and

$$N^{(e)} = \sum_{j=1}^{q_e} N_j^{(e)} = \exp\gamma_e \sum_{j=1}^{q_e} g_j^{(e)} \exp(\beta\epsilon_i^{(e)}) \tag{12}$$

for $e = s+1, s+2, \cdots, s+m$. The partition function Q_l for the lth specie is defined as

$$Q_l = \sum_{j=1}^{q_l} g_j^{(l)} \exp(\beta\epsilon_j^{(l)}) \tag{13}$$

where the undetermined Lagrangian multiplier β is $(-1/kT)$. Expressions of the type of Eqs. (11) and (12) can be combined to eliminate the remaining undetermined Lagrangian multipliers $\gamma_{s+1}, \gamma_{s+2}, \gamma_{s+3}, \cdots, \gamma_{s+m}$ and yield

$$\frac{N^{(i)}}{\prod_{j=s+1}^{s+m} (N^{(j)})^{\alpha_{ij}}} = \frac{Q_i}{\prod_{j=s+1}^{s+m} (Q_j)^{\alpha_{ij}}} \tag{14}$$

or for

$$n^j = \frac{N^j}{AV}$$

where V is the volume of the mixture and A is Avagadro's number.

$$\frac{n^{(i)}}{\prod_{j=s+1}^{s+m} (n^{(j)})^{\alpha_{ij}}} = \frac{\left(\frac{Q_i}{VA}\right)}{\prod_{j=s+1}^{s+m} \left(\frac{Q_j}{VA}\right)^{\alpha_{ij}}} \tag{15}$$

for $i = 1, 2, 3, \cdots, s$. Equations of the type of Eq. (15) are identical to the "equations of mass action" given in Ref. 1 providing

$$-\frac{f_i^o}{RT} = \ln(RT) + \ln\left(\frac{Q_i}{VA}\right) \tag{16}$$

Furthermore, from the integral of Eq. (7), the specific enthalpy can be shown to be

$$\frac{h_i^o}{RT} = 1 + \frac{\sum_{j=1}^{g_i} \frac{\epsilon_i}{KT} \exp\left(-\frac{\epsilon_i}{KT}\right)}{Q_i} = 1 + KT\left(\frac{\partial \ln(Q_i)}{\partial KT}\right)_V \tag{17}$$

The other constraints on the concentrations supplied by the conservation of mass of chemical elements require that

$$n_j = \sum_{i=1}^{s} \alpha_{ij} n_i = B_j \rho/\rho_o \tag{18}$$

for $j = s+1, s+2, s+3, \cdots, s+m$ where

B_j = concentration of the jth element at standard temperature and pressure; and

ρ_o = density of the mixture at standard temperature and pressure.

Equation (18) is frequently referred to as the "equation of mass balance." The solution of the s mass action equations and the m mass balance equations for a given temperature, density, and concentration of elements at standard conditions is a set of $s + m$ concentrations which satisfy the criterion of chemical equilibrium.

After the equilibrium concentrations have been determined, the thermodynamic properties of the gaseous mixture are calculated by the following relations:

$$n = \sum_{i=1}^{s+m} n_i$$

$$P = nRT$$

$$H = \frac{\sum_{i=1}^{s+m} n_i h_i^o}{\rho} \tag{19}$$

$$Z = \frac{\frac{P}{\rho RT}}{\frac{P_o}{\rho_o RT_o}} = \frac{M_o}{M}$$

$$\frac{SM_o}{R} = \frac{M_o}{\rho} \sum_{i=1}^{s+m} n_i \left(\frac{h_i^o - f_i^o}{RT} - \ln P - \ln \frac{n_i}{n}\right)$$

The quantities which appear above are defined as:

h_i^o	specific enthalpy of the ith constituent at one atmosphere
M_i	molecular weight; whether in lb/lb-mole or g/g-mole, the values are identical
M_o	molecular weight of mixture at STP
n	total concentration of mixture, moles/liter
n_i	concentration of the ith constituent
R	universal gas constant = 1.9860 Btu/°R-lb-mole = 1.98726 cal/°K-g-mole
S	entropy
$\frac{SM_o}{R}$	dimensionless entropy
T	temperature
T_o	standard temperature = 273.15°K
ρ	mass density

III. Normal Shock Problem

From the aerothermodynamic point of view, one of the most important yet simplest applications of the chemical equilibrium data described above is the normal shock problem. The equations governing the variation of properties through a normal shock, when the coordinate system is chosen so the flow is steady and one dimensional,

and when the effects of body forces, diffusion, and radiative transfer are negligible, are:
continuity:

$$\frac{d}{dx}(\rho U) = 0 \tag{20}$$

linear momentum:

$$\rho U \frac{dU}{dx} + \frac{dP}{dx} = \tfrac{4}{3}\frac{d}{dx}\left(\eta \frac{dU}{dx}\right) \tag{21}$$

and *energy:*

$$\rho U \frac{dE}{dx} + P\frac{dU}{dx} = \frac{d}{dx}\left(K\frac{dT}{dx}\right) + \tfrac{4}{3}\eta\left(\frac{dU}{dx}\right)^2 \tag{22}$$

Integration of these equations with respect to x yields

$$\rho U = C_1 \tag{23}$$

$$\rho U^2 + P = \tfrac{4}{3}\eta\frac{dU}{dx} + C_2 \tag{24}$$

$$\rho U\left(H + \frac{U^2}{2}\right) = \left(K\frac{dT}{dx} + \tfrac{4}{3}\eta U\frac{dU}{dx}\right) + C_2 \tag{25}$$

where C_1, C_2, and C_3 are constants. If these equations are applied across a normal shock, and if either: (1) the fluid is assumed to be inviscid ($\eta = 0$) and nonheat-conducting ($K = 0$), or (2) the fluid is assumed to be in thermodynamic equilibrium (i.e., the gradients are zero), then the equations reduce to the form

$$\rho_A U_A = \rho_B U_B \tag{26}$$

$$\rho_A U_A^2 + P_A = \rho_B U_B^2 + P_B \tag{27}$$

$$H_A + \frac{U_A^2}{2} = H_B + \frac{U_B^2}{2} \tag{28}$$

Therefore, Eqs. (26), (27), and (28) relate the thermodynamic properties and velocities in the up-stream and down-stream equilibrium regions of the flow field associated with a standing normal shock as shown in Fig. 1.

Three special applications of Eqs. (26), (27), and (28) to the equilibrium regions of shock flows are (1) the moving shock problem, (2) the standing shock problem, and (3) the reflected shock problem.

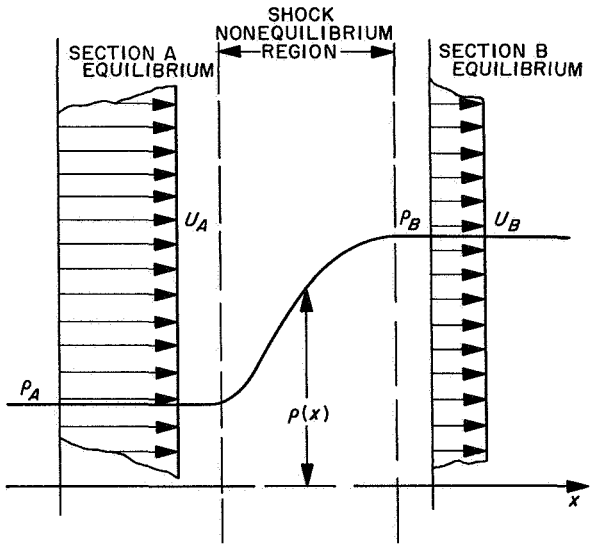


Fig. 1. Flow field associated with a normal shock

A. Free-Flight or Moving Shock Case

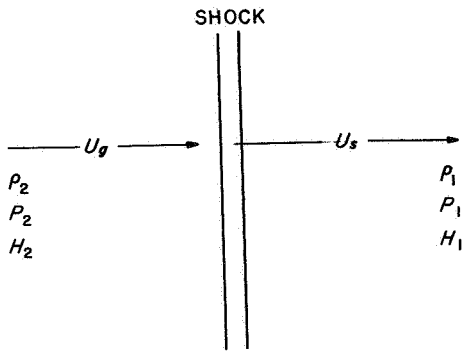
The free-flight or moving shock problem is of interest for determining the velocities and thermodynamic properties behind the normal portion of the bow shock associated with a high velocity blunt body. The free-flight problem is equivalent to the moving shock problem in a shock tube. Physically, the problem is the determination of the properties behind a shock which is propagating in quiescent gas at a specified velocity. Mathematically, the problem is to satisfy the Hugoniot equation,

$$H_B - H_A = \tfrac{1}{2}(P_B - P_A)\left(\frac{1}{\rho_A} + \frac{1}{\rho_B}\right) \tag{29}$$

which is obtained from a suitable manipulation of Eqs. (26), (27), and (28). The initial properties H_A, P_A, and ρ_A are known, and the chemical equilibrium computation yields relations for $H_B(\rho_B, T_B)$ and $P_B(\rho_B, T_B)$. Thus, by selecting one property in region (B), the other properties are determined by Eq. (29). The Hugoniot equation and the auxiliary equations are shown in Figs. 2 and 3 with subscripts appropriate to the free-flight and moving shock problems.

B. Standing Shock Case

The standing shock situation considered here results from the flow of the high-velocity, high-enthalpy gas associated with the above mentioned moving normal shock case over a stationary blunt body. The flow around the body is such that a stationary bow shock develops.



EQUATIONS TO BE SATISFIED:

$$H_2 - H_1 = \tfrac{1}{2}(P_2 - P_1)\left(\frac{1}{\rho_1} + \frac{1}{\rho_2}\right) \quad (30)$$

$$U_s = \sqrt{\frac{\rho_2}{\rho_1}\left(\frac{P_2 - P_1}{\rho_2 - \rho_1}\right)} = \text{SHOCK VELOCITY,} \quad (31)$$

$$U_g = U_s\left(1 - \frac{\rho_1}{\rho_2}\right) = \text{GAS VELOCITY} \quad (32)$$

Fig. 2. Moving normal shock

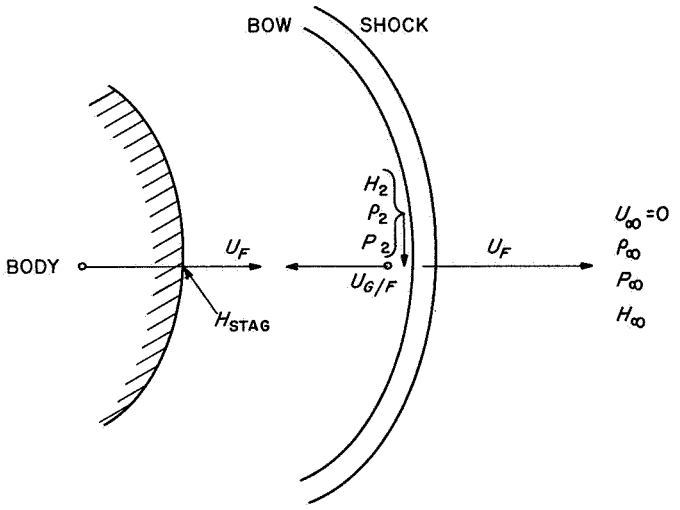
Physically, the problem is one of determining the properties and velocity in the equilibrium region immediately behind the bow shock. The important thermodynamic properties and velocities are indicated in Fig. 4.

Also shown in this figure are the appropriate forms of Eqs. (26), (27), and (28) which for known U_g, ρ_2, H_2, P_2 and the implicit chemical equilibrium property relations $H_3(T_3, \rho_3)$ and $P_3(T_3, \rho_3)$ allow the velocities and state of the gas behind the standing shock to be determined. The results of this type of calculation are useful in shock tube simulation of entry conditions.

C. Reflected Shock Case

The third problem of interest, the reflected shock case, results from the stagnation of the high-velocity, high-enthalpy gas of a moving shock by an immovable plane surface. The gas comes to rest by means of a reflected shock which propagates into the gas flowing toward the surface.

The thermodynamic properties and velocities are defined in Fig. 5 along with the equations to be satisfied. Other than a slightly different form of the equations, the mathematical problem here is equivalent to the standing shock case described earlier. The results of this type of calculation are useful in interpreting experiments performed at the end of a shock tube.



EQUATIONS TO BE SATISFIED:

$$H_2 - H_\infty = \tfrac{1}{2}(P_2 - P_\infty)\left(\frac{1}{\rho_\infty} + \frac{1}{\rho_2}\right) \quad (33)$$

$$U_F = \sqrt{\frac{\rho_2}{\rho_\infty}\left(\frac{P_2 - P_\infty}{\rho_2 - \rho_\infty}\right)} = \text{FLIGHT VELOCITY} \quad (34)$$

$$U_{G/F} = \sqrt{\frac{\rho_\infty}{\rho_2}\left(\frac{P_2 - P_\infty}{\rho_2 - \rho_\infty}\right)} = \text{VELOCITY OF GAS RELATIVE TO THE BODY} \quad (35)$$

$$H_{STAG} = H_2 + \tfrac{1}{2} U_{G/F}^2 = \text{STAGNATION ENTHALPY} \quad (36)$$

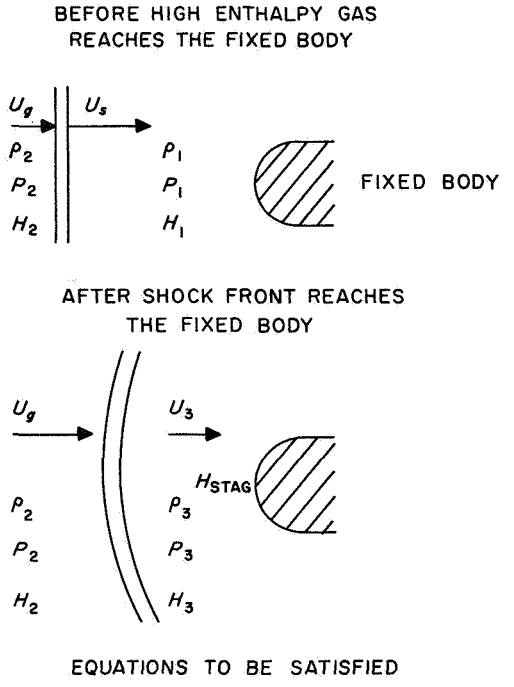
Fig. 3. Free-flight bow shock

Before considering the numerical techniques used to satisfy the chemical equilibrium and shock equations, it is important to emphasize that the above equations closely approximate shock-tube and free-flight conditions only where the shock heated gas is in chemical equilibrium and the effect of wall shear and heat transfer is small.

IV. Numerical Procedure

A. Chemical Equilibrium

To obtain the $s + m$ constituents of a gaseous mixture in chemical equilibrium requires the simultaneous solution of the m mass balance equations and the s nonlinear mass action equations. The Newton-Raphson method is well suited for solving such a system of simultaneous algebraic equations with a high-speed digital computer. The Newton-Raphson method applied to the present problem allows a solution to be obtained by an iterative



EQUATIONS TO BE SATISFIED

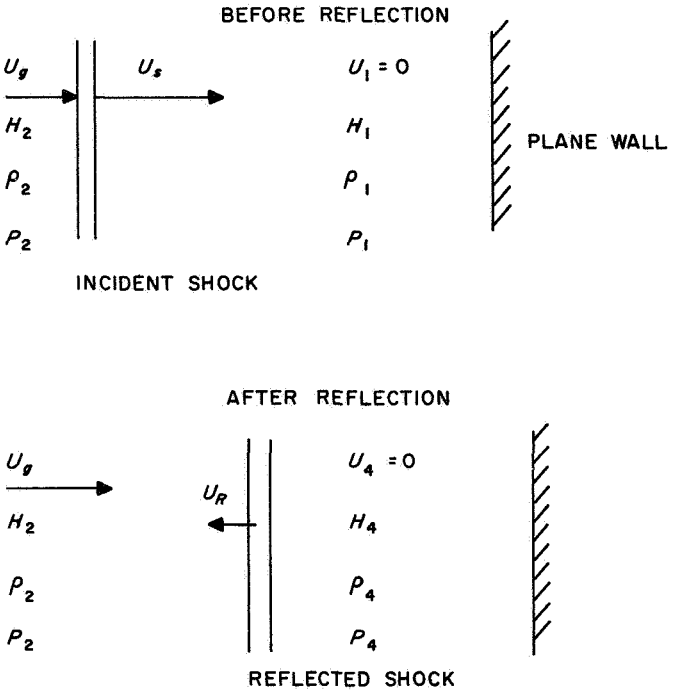
$$H_3 = H_2 + \frac{U_g^2}{2}\left[1 - \left(P_2/P_3\right)^2\right] \tag{37}$$

$$P_3 = P_2 + \rho_2 U_g^2\left[1 - P_2/P_3\right] \tag{38}$$

$$U_3 = \left(P_2/P_3\right)U_g \tag{39}$$

$$H_{STAG} = H_3 + \frac{U_3^2}{2} \tag{40}$$

Fig. 4. Standing shock case



EQUATIONS TO BE SATISFIED:

$$H_4 = H_2 + \frac{U_g^2}{2}\left(\frac{\rho_4/\rho_2 + 1}{\rho_4/\rho_2 - 1}\right) \tag{41}$$

$$P_4 = P_2 + \rho_2 U_g^2\left(\frac{\rho_4/\rho_2}{\rho_4/\rho_2 - 1}\right) \tag{42}$$

$$U_R = \frac{U_g^2}{\rho_4/\rho_2 - 1} = \text{REFLECTED SHOCK VELOCITY} \tag{43}$$

Fig. 5. Reflected shock case

procedure which involves solving a linearized form of Eqs. (15) and (18). The method assumes that a point defined by a set of concentrations which nearly satisfy the mass action and mass balance conditions is known. By expanding the mass action and mass balance equations in a Taylor series about the near solution point and neglecting terms of the series which contain derivatives higher than the first order, a system of linear equations is obtained which approximate the mass action and mass balance equations. The solution of the linear system of equations results in a new set of concentrations which are nearer the actual solution to the mass action and the mass balance equations. Clearly, by repeating this procedure, a better set of concentrations can be found so that by iterating enough times a solution with any desired accuracy can be found. With a high-speed digital computer this procedure is quite simple, fast, and accurate.

The linearized form of the mass action (Eq. 15) and mass balance (Eq. 18), obtained from the series expansion with the temperature, density, and initial molar concentration constant, is of the following form:

(1) Mass action.

$$(Z_k)_{p+1} - \sum_{j=s+1}^{s+m} \alpha_{kj}\,(Z_j)_{p+1} + (D_k)_p = 0 \tag{44}$$

where

$$k = 1, 2, 3, \cdots, s$$

$(\ )_p$ = indicates value from the pth iteration

$$(D_k)_p = \ln (n_k)_p + \ln RT + \frac{f_k^o}{RT}$$

$$- \sum_{j=s+1}^{s+m} \alpha_{kj} \left[\ln (n_j)_p + \ln RT + \frac{f_j^o}{RT} \right]$$

(2) Mass balance.

$$(n_j)_p (Z_j)_{p+1} + \sum_{k=1}^{s} \alpha_{kj} (n_k)_p (Z_k)_{p+1} + (D_j)_p = 0 \qquad (45)$$

where

$$j = s+1, s+2, s+3, \cdots, s+m$$

and

$$(D_j)_p = (n_j)_p + \sum_{k=1}^{s} \alpha_{kj} (n_k)_p - \frac{B_j \rho}{\rho_o}$$

In the above expressions,

$$(Z_i)_{p+1} = \ln (n_i)_{p+1} - \ln (n_i)_p$$

The use of the natural logarithm of the concentration as the variable in the series expansion was suggested in Ref. 40 and was found to give good results.

This linear system of $s+m$ equations can be simplified to m equations by using Eq. (44) to eliminate $Z_1, Z_2, Z_3, \cdots, Z_s$ from Eq (45). The result of this substitution is a system of m linear equations of the form:

$$\sum_{j=1}^{m} (Y_{ij})_p (Z_{s+j})_{p+1} = (C_i)_p \qquad (46)$$

where $i = 1, 2, 3, \cdots, m$. The quantities Y_{ij} and C_i are given by

$$(Y_{ij})_p = \delta_{ij} (n_{s+i})_p + \sum_{k=1}^{s} (n_k)_p (\alpha_{k,s+1}) (\alpha_{k,s+1})$$

$$\delta_{ij} = 0 \qquad \text{for } i \neq j$$

$$\delta_{ij} = 1 \qquad \text{for } i = j$$

and

$$(C_i)_p = - \left[(D_{s+i})_p - \sum_{k=1}^{s} (n_k)_p (D_k)_p (\alpha_{k,s+1}) \right]$$

To use Eq. (46) in obtaining a solution to Eqs. (15) and (18), the following procedure is used:

(1) Using initial guesses, $(n_1)_o, (n_2)_o, (n_3)_o, \cdots, (n_{s+m})_o$, for the concentrations at a selected temperature, density, and concentration of chemical elements at standard conditions, the coefficients $(D_i)_o$ and $(Y_{ij})_o$ are evaluated.

(2) A solution to the system of Eq. (46) is found using the Crout method. The solution

$$(Z_{s+1})_1, (Z_{s+2})_1, (Z_{s+3})_1, \cdots, (Z_{s+m})_1$$

yields values for

$$(n_{s+1})_1, (n_{s+2})_1, (n_{s+3})_1, \cdots, (n_{s+m})_1$$

(3) The $(n_1)_1, (n_2)_1, (n_3)_1, \cdots, (n_s)_1$ are evaluated using Eq. (44).

(4) The new values of the concentration $(n_i)_1$ with $i = 1, 2, 3, \cdots, s+m$ replace the initial guesses, and the above procedure is repeated k times until

$$1 - \left| \frac{(n)_k}{(n)_{k+1}} \right| < 10^{-6}$$

and

$$1 - \left| \frac{(\rho)_k}{(\rho)_{k+1}} \right| < 10^{-6}$$

and

$$1 - \left| \frac{(\bar{H})_k}{(\bar{H})_{k+1}} \right| < 10^{-6}$$

where

$(\ )_{k+1}$ = value from the $(k+1)$ iteration

n = total concentration

ρ = density of mixture

$\bar{H}$ = enthalpy per unit volume

This convergence criterion has been found to result in a set of concentrations $(n_1)_{k+1}, (n_2)_{k+1}, (n_3)_{k+1}, \cdots, (n_{s+m})_{k+1}$ which agree with $(n_1)_k, (n_2)_k, (n_3)_k, \cdots, (n_{s+m})_k$ to at least three significant figures.

B. Moving and Free-Flight Normal Shock Case

The moving shock problem, as discussed earlier, consists of finding a thermodynamic state defined by T_2 and

ρ_2 which satisfies the Hugoniot equation for specified initial conditions. The initial conditions are specified by the pressure, temperature, and concentrations. To find a final state which satisfies the Hugoniot equation, a final temperature T_2 is specified and the value of ρ_2 is varied until values of p_2 and H_2 are found which satisfy the Hugoniot equations. After the properties which satisfy the Hugoniot equations are found, the Eqs. (31), (32), (34), (35), and (36) are evaluated.

The systematic procedure for finding the correct value of ρ_2 is based on a Newton-Raphson iteration scheme in which the Hugoniot equation

$$F(v_2, T_2) = [H_2(v_2, T_2) - H_1] - \tfrac{1}{2}[P_2(v_2, T_2) - P_1]\left[\frac{1}{\rho_1} + v_2\right] \tag{47}$$

is expanded in v_2 at some near solution point with T_2 held constant. The resulting iteration relation for the nth iteration is

$$(v_2)_{n+1} = \left(\frac{1}{\rho_2}\right)_{n+1} = \left(\frac{1}{\rho_2}\right)_n - \frac{F((v_2)_n, T_2)}{\left(\left.\frac{\partial F}{\partial v_2}\right|_{T_2}\right)_n} \tag{48}$$

where the partial derivative is evaluated by

$$\left(\left.\frac{\partial F}{\partial v_2}\right|_{T_2}\right)_n = \frac{F((v_2)_n + (\Delta v_2)_n, T_2) - F((v_2)_n, T_2)}{\Delta v_2}$$

with

$$(\Delta v_2)_n = 10^{-6}(v_2)_n$$

The Hugoniot equation is considered satisfied after n iterations if:

$$\left|\frac{(1/\rho_2)_{n+1} - (1/\rho_2)_n}{(1/\rho_2)_n}\right| \leq 10^{-3}$$

C. Reflected and Standing Normal Shock Cases

The procedures followed for the reflected shock case and the standing shock case are similar. Therefore, only the reflected shock case will be discussed below.

The problem in the reflected shock case is to find a T_4 and ρ_4 associated with values of H_4 and P_4 which satisfy Eqs. (41) and (42). The values of H_2, ρ_2, P_2, and U_g are known from the moving normal shock solution.

The solution technique is based upon a series expansion of the thermodynamic properties H and P about some point (T_a, ρ_a) which is near (T_4, ρ_4). The truncated series are of the form

$$H = H_a + \left.\frac{\partial H}{\partial \rho}\right|_a \delta\rho + \left.\frac{\partial H}{\partial T}\right|_a \delta T \tag{49}$$

$$P = P_a + \left.\frac{\partial P}{\partial \rho}\right|_a \delta\rho + \left.\frac{\partial P}{\partial T}\right|_a \delta T \tag{50}$$

with

$$\delta\rho = \rho - \rho_a$$

$$\delta T = T - T_a$$

Equations (41) and (42) are functions of ρ_4. By evaluating these equations at $\rho_4 = \rho_a$, approximate values of H_4 and P_4 result. Substituting these approximate values (H_4' and P_4') into the left-hand side of Eqs. (49) and (50), and combining so that δT is eliminated, yields

$$\delta\rho = \frac{(H_4' - H_a)\left.\frac{\partial P}{\partial T}\right|_a - (P_4' - P_a)\left.\frac{\partial H}{\partial T}\right|_a}{\left.\frac{\partial P}{\partial T}\right|_a \left.\frac{\partial H}{\partial \rho}\right|_a - \left.\frac{\partial P}{\partial \rho}\right|_a \left.\frac{\partial H}{\partial T}\right|_a} \tag{51}$$

The partial derivatives are evaluated by the finite difference relations

$$\left.\frac{\partial P}{\partial T}\right|_a = \frac{P(T_a + \Delta T, \rho_a) - P(T_a, \rho_a)}{\Delta T}$$

$$\left.\frac{\partial H}{\partial T}\right|_a = \frac{H(T_a + \Delta T, \rho_a) - H(T_a, \rho_a)}{\Delta T}$$

$$\left.\frac{\partial H}{\partial \rho}\right|_a = \frac{H(T_a, \rho_a + \Delta\rho) - H(T_a, \rho_a)}{\Delta\rho}$$

$$\left.\frac{\partial P}{\partial \rho}\right|_a = \frac{P(T_a, \rho_a + \Delta\rho) - P(T_a, \rho_a)}{\Delta\rho}$$

where $\Delta\rho/\rho = 10^{-4}$ and $\Delta T = 500°K$. The 500°K increment was found to give the best results.

Now, the value of $\delta\rho$ obtained from the evaluation of Eq. (51) yields a density $(\rho)_{n+1} = (\rho)_n + \delta\rho$ which is closer to the desired value ρ_4. By reevaluating the quantities in the right-hand side of Eq. (51) at the new value of density, further improvements result. When

$$\frac{(\delta\rho)_n}{(\rho_4)_n} \leq 10^{-3}$$

the value of $(\rho_4)_{n+1}$ is considered to be a solution. Using this value for ρ_4, the values of H_4 and P_4 are evaluated using Eqs. (41) and (42), and the value of T_4 is obtained from Eq. (49). Once convergence is achieved, equilibrium computations are performed at the values of T_4 and ρ_4 to obtain the actual chemical concentrations and properties at the solution point.

V. Program Description

The numerical solution procedures discussed earlier have been programmed so that the following combinations of problem cases can be considered:

(1) *The Mollier data case* in which the program calculates the chemical equilibrium properties and composition of a gaseous mixture of specified temperature, density, and initial composition. The computation takes about 2 s* per temperature-density point.

(2) *The moving normal shock case* in which the program calculates the properties of a moving shock when the temperature (T_2), initial temperature (T_1), pressure (P_1), and chemical composition are specified. The computer requires about 5 s for each solution.

(3) *A combination case* in which the normal moving shock case is first solved and then a solution for the resulting *standing shock* is obtained. The shock parameters and chemical compositions for both situations make up the output for this case. The time required for this case is 20 s per moving shock.

(4) *A combination case* in which the normal moving shock case is first solved and then a solution for the resulting *reflected shock* is obtained. The shock parameters and chemical compositions for both situations makes up the output data. The time requirement for this case is identical to that of (3) above.

(5) *A combination case* in which the normal moving shock solution is first obtained, then *both standing* and *reflected solutions* are generated. The shock parameters and chemical compositions for all three conditions of thermodynamic equilibrium are printed out. This case takes 45 s per moving normal shock.

*The computation time is dependent upon the number of species. The times quoted in the five cases are for problems having 20 species in the final composition. As an example of this time dependence in the moving-standing-reflected shock combination case, the computation takes 15 s when 10 species are used, 45 s for 20 species, and 2 min for 40 species.

The program has sufficient capacity to store in its library data up to 130 chemical species. Of these, 32 can be atomic or atomic ions, 20 can be diatomic species, and 75 can be polyatomic species. The other species are the double-ionized helium, the proton for ionized hydrogen, and the electron. These above limitations are somewhat arbitrary and may be modified by simply changing dimension statements in the program providing storage capacity is available in the computer system. The program library consists primarily of spectroscopic data from which the energy levels of the various species can be deduced.

These library data are used by a thermochemical property subroutine to compute the partition functions and subsequently the specific free energies and enthalpies. In this way the program can be updated as more precise energy-level or heat-of-formation data become available. Also, the use of a subroutine allows the procedure used in computing the partition functions to be changed with ease. The subroutine and the problems in computing partition functions are discussed in an accompanying report (Ref. 38).

Also, to allow easy modification of the output format, the output data for all five cases are handled by a common subroutine.

The gross features and logic of the program are shown in Fig. 6. For a detailed description, the flow diagram and program listing in Appendices B and D, respectively, should be helpful.

VI. Program Input

The input data for the program is divided into two decks. The first deck, referred to as "library data," contains the data from which thermochemical properties (specific enthalpy and free energy) for each chemical species can be computed using the techniques of statistical mechanics. The entire library data deck is read into the machine following the program deck.

The second deck of input data, referred to as "case data," is used to identify the particular case (i.e., Mollier data, moving normal shock, or combined normal shock), to specify which species of the library data constitute the mixture, and to specify certain initial and final state conditions. This division of the input data into two parts allows the thermochemistry data in the library to be used without rearrangement or modification, while making it accessible for modification if better values become available. The order of the program deck, library data deck, and case data decks is shown in Fig. 7.

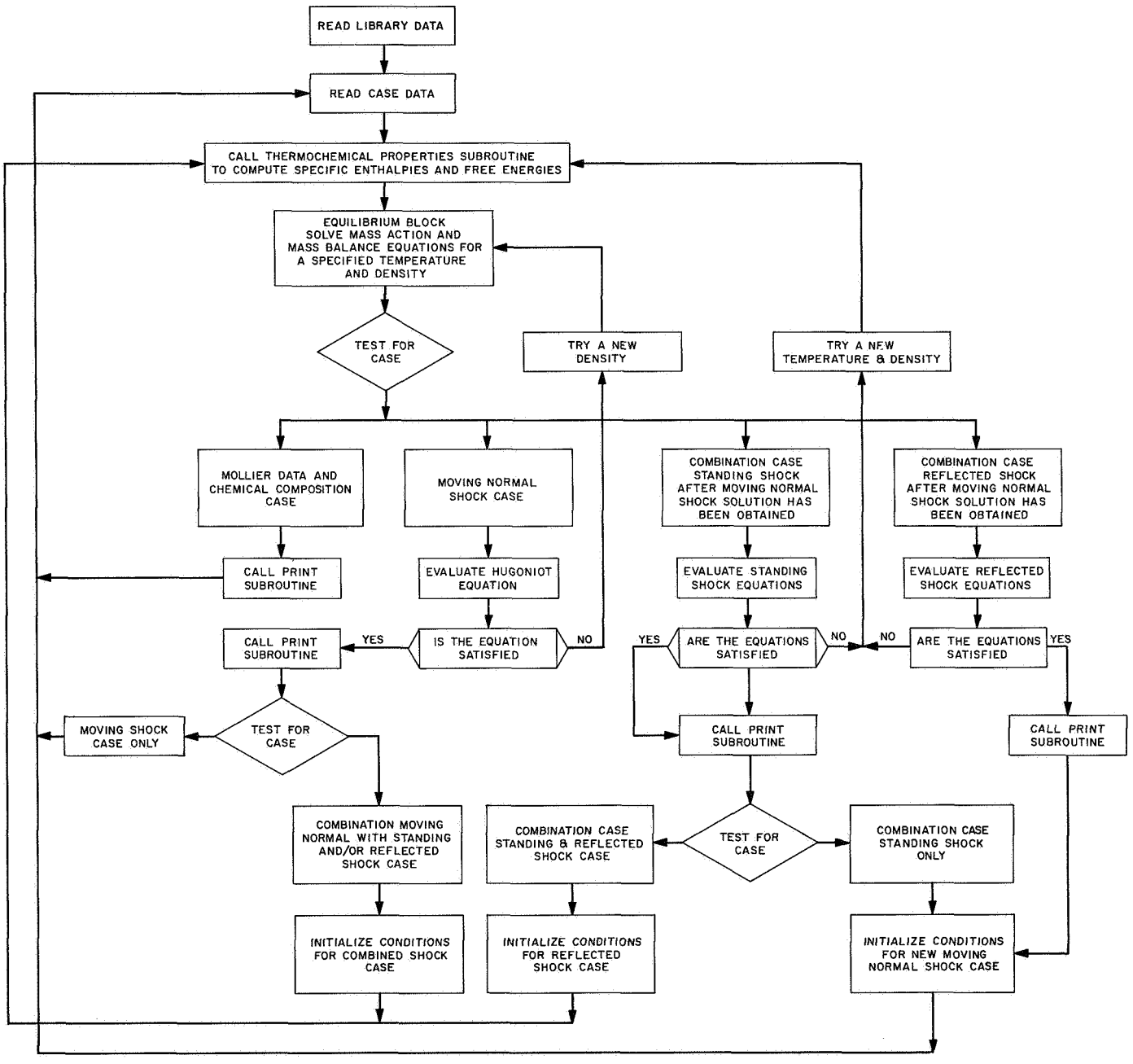


Fig. 6. Flow diagram for the program

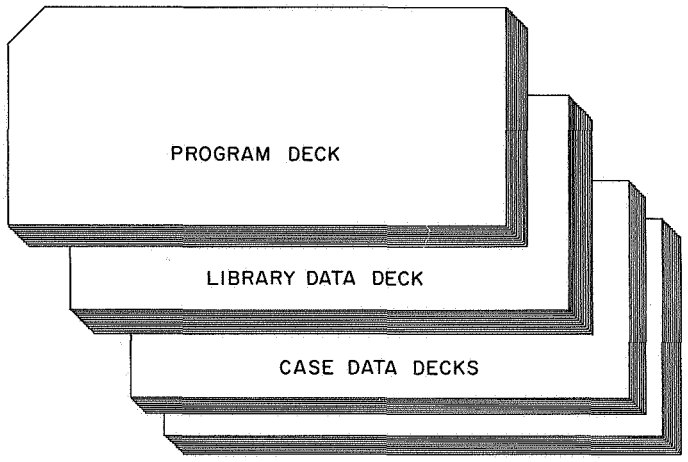


Fig. 7. Order of the program and data decks

A. Library Data

The library data deck consists of packets of cards for each species which contain the formula vector, molecular weight, heat of formation, and sufficient information about the structure and energy states to allow one to compute the partition function and the specific enthalpy and free energy. Because the information used to represent the energy states and structure as well as the details of the above computation for atomic species is quite different from that for diatomic species, each library data packet takes one of five different forms. The form or format for four of these—(1) atomic or atomic ion, (2) diatomic molecule or ion, (3) linear polyatomic molecule, and (4) nonlinear polyatomic molecule—is given in Table 1. The fifth type of species contains those particles which lack internal structure. For the energy range considered here, these are the electron, the proton or hydrogen positive ion, and the helium double-positive ion. Each of the packets is assigned a library identification number which corresponds to the position of the packet in the deck. The identification number is for the user's convenience as the computer does not read it but assigns identification numbers based upon the order of the packet in the deck. Thus, if the order of deck is changed by adding or deleting or rearranging packets, the packets should be renumbered so that they can be properly identified. The only constraint on the order of the packets is that those species used as "components" of the formula vectors be listed last and in an order such that the matrix of their formula vectors is a unitary matrix. For illustrative purposes, we

Table 1. Example data packets

A. Atomic and atomic ions

11 C++ 1 0 0 0 0—2 12.01005 01 20 0.0			Specie identification card
C++ HEAT FORMATION 0.991689E 03			Heat of formation card
CIII	1.00	0.0	
CIII	5.00	52394.797	
CIII	4.00	52338.000	
CIII	3.00	102351.375	
CIII	9.00	137450.500	
CIII	5.00	145875.062	
CIII	1.00	182520.187	
CIII	4.00	238160.687	
CIII	12.00	259672.062	
CIII	15.00	269962.875	
CIII	5.00	276482.687	Energy level block
CIII	12.00	308264.750	
CIII	16.00	317748.000	
CIII	78.00	321964.687	
CIII	49.00	333395.000	
CIII	116.00	346526.000	
CIII	90.00	358639.000	
CIII	29.00	365585.000	
CIII	39.00	373748.000	
CIII	37.00	381958.000	

Table 1 (contd)

B. Diatomic

21	N2+	0	2	0	0	0—1				28.016	02	4	2.0			Specie identification card
N2+	HEAT FORMATION	0.359306E	03													Heat of formation card
N2+	X DOUBLET SIGMA				0.0		2207.23		16.22		1.9322		0.0202		2.0	Energy level block
N2+	A DOUBLET PI				9020.0		1902.84		14.91		1.722		0.018		4.0	
N2+	B DOUBLET SIGMA				25570.0		2419.84		23.19		2.083		0.0195		2.0	
N2+	C DOUBLET SIGMA				64550.0		2050.0		14.92		1.65		0.05		2.0	

C. Linear polyatomic

07	C02	1	0	2	0	0	0	0	0	0	0	44.011	03	4	0.0	Specie identification card
C02	HEAT FORMATION	—.939643E+02														Heat of formation card
C02	SINGLET SIGMA	2.01.0	0.3906	0.0022	4											Energy level block
667.33																
667.33																
1342.86																
2349.3																

D. Non-linear polyatomic

05	N02	0	1	2	0	0	0	0	0	0	0	46.008	04	3	0.0	Specie identification card
N02	HEAT FORMATION	0.876600E+01														Heat of formation card
N02					2.02.0	3.47500E—4063.54500E—4067.02000E—4003										Energy level block
N02					756.8											
N02					1357.8											
N02					1665.5											

will consider an arrangement of the library data packets as given in Table 2. A more extensive list of library data is given in Appendix E.

The library data are arranged with Card No. 1 first, followed by the species data packets. The species data packets consist of a first card which is called the species identification card, a heat of formation card, and the energy level block.

1. Card No. 1

The information on Card No. 1 is in format 2I2.** The first word on this card gives the number of chemical components or elements, plus the electron, which are listed in the library. The second word is the total number of species in the library. For the sample listing in Table 2, the first card would contain 05 in the first two columns, since C, N, O, e, A are present, and 36 in the second two columns.

2. Data Packets

Specie Identification Card: The first card of each packet contains in the following order:

(1) The specie identification number.

(2) The chemical formula.

(3) The α_{ij}'s of the formula vector.

(4) The molecular weight.

(5) The specie type number (01 for atomic or atomic ions, 02 for diatomic species, 03 for linear polyatomic species, 04 for non-linear polyatomic species, and 05 for electrons, H^+, and He^{++}).

**Pertinent format notation is given in Appendix C.

Table 2. Sample library data list

ID No. i	Formula	Formula vector				
		$\alpha_{i,32}$	$\alpha_{i,33}$	$\alpha_{i,34}$	$\alpha_{i,35}$	$\alpha_{i,36}$
1	CN	1	1	0	0	0
2	NO^+	0	1	1	−1	0
3	CO	1	0	1	0	0
4	NO	0	1	1	0	0
5	NO_2	0	1	2	0	0
6	N_2O	0	2	1	0	0
7	CO_2	1	0	2	0	0
8	N_2	0	2	0	0	0
9	O_2	0	0	2	0	0
10	C^{+++}	1	0	0	−3	0
11	C^{++}	1	0	0	−2	0
12	C^+	1	0	0	−1	0
13	C^-	1	0	0	1	0
14	CO_+	1	0	1	−1	0
15	C_2N_2	2	2	0	0	0
16	C_2	2	0	0	0	0
17	C_3	3	0	0	0	0
18	N^{+++}	0	1	0	−3	0
19	N^{++}	0	1	0	−2	0
20	N^+	0	1	0	−1	0
21	N_2^+	0	2	0	−1	0
22	O^{+++}	0	0	1	−3	0
23	O^{++}	0	0	1	−2	0
24	O^+	0	0	1	−1	0
25	O^-	0	0	1	1	0
26	O_2^-	0	0	2	1	0
27	O_2^+	0	0	2	−1	0
28	O_3	0	0	3	0	0
29	A^{+++}	0	0	0	−3	1
30	A^{++}	0	0	0	−2	1
31	A^+	0	0	0	−1	1
32	C	1	0	0	0	0
33	N	0	1	0	0	0
34	O	0	0	1	0	0
35	e	0	0	0	1	0
36	A	0	0	0	0	1

(6) The number of energy levels (for atomic and ionic species, this will be the number of energy level cards which make up the packet and cannot exceed 70; for diatomic species, this will be the number of electronic state cards which make up the packet and can not exceed 10; for linear polyatomic or nonlinear polyatomic species, this will be the number of vibrational frequency cards which make up the packet and cannot exceed 12; for the electron H^+ and He^{++}, this number is zero).

(7) The last number on the card is zero for all species except the diatomic forms. For homo-nuclear diatomic molecules, the value is 2.0; for unlike nuclei, the value is 1.0. This is a symmetry number for diatomic species.

The format of this card is 12X, A6, 10I2, 1F10.6, I2, I4, 1F4.1. The column positions of the items listed above are shown in Table 1.

Heat of Formation Card: The second card of each packet contains the value of the heat of formation, h_o^o, in kcal/mole for the species associated with the packet. The format of this card is 20X, 1E12.6.

Energy Level Block Cards of Atomic Species: The energy level block for atomic or ionic species consists of a tabulation of the electronic energy levels of the ground and excited states together with the degeneracy of these levels. One degeneracy, g_i, and one energy level, E_i, in units of cm^{-1} are listed on each card. The cards are arranged with the ground state first and with successive excited states following. The format for each card is 19X, 1F6.2, 3X, 1F10.3. The number of these cards in each packet should correspond to the number listed in the next to last position on the species identification card for the species. The total number of these cards in each atomic or ionic species data packet should not exceed 70. Provision has been made for 32 atomic and atomic ion data packets.

Energy Level Block Cards of Diatomic Species: The energy level block for diatomic species consists of a tabulation of the electronic energy levels of the ground and excited states together with the degeneracy and the vibrational and rotational constants for these levels. The first 25 columns of each card are not read by the machine so they can be used for identification. Each card represents an electronic level and contains the electronic energy term, T_e; the vibrational frequency term, ω_e; the anharmonic term, $\omega_e x_e$; the rotational term, B_e; the vibrational-rotational coupling term, α_e; and last, the degeneracy of the electronic energy level, p. The term values are in units of cm^{-1}. The cards are arranged with the ground level first followed by the successive excited states. The format of each card is 25X, 1F11.4, 1F9.3, 1F10.5, 1F10.6, 1F9.6, 1F6.2. The number of cards in each packet should correspond to the number listed in the next to last position on the species identification card for the packet. The total number of these cards in each diatomic species data packet should not exceed 10. Provision has been made for 20 diatomic data packets.

Energy Level Block Cards of Linear Polyatomic Species: The energy level block for linear polyatomic species contains the information necessary to describe the rotational-vibrational energy states of the ground electronic configuration of the molecule. The first 25 columns

of the first card of this block are not read by the computer and may be used for identification. The format of this card is 25X, 2F3.1, 2F8.5. The first word on the card is the symmetry number for the molecule, σ, followed by the degeneracy of the electronic ground state, p; the rotational terms B_e and α_e are in units of cm^{-1}. The last item on this card which is not read is the number of vibrational degrees of freedom for the molecule for which frequencies, ω, (cm^{-1}) are tabulated on successive cards in 1F8.2 format. The above number should also be listed in the next to last position on the species identification card for the packet. The total number of vibrational degrees of freedom should not exceed 12. The total combined number of linear and nonlinear polyatomic atomic data packets can not exceed 75.

Energy Level Block Cards of Non-Linear Polyatomic Species: The energy level block for non-linear polyatomic molecules contains the information necessary to describe the rotational-vibrational energy states of the ground electronic configuration. The first 25 columns of the first card of this block are not read and can be used for identification. The format is 25X, 2F3.1, 1F8.5, 4X, 1F8.5, 4X, 1F8.5. The first two words are the symmetry number, σ, and degeneracy of the electronic ground state, p. The other items on the card are the three moments of inertia (I_x, I_y, I_z) for the molecule. These should be in units of gm-$cm^2 \times 10^{40}$ as the "$E - 40$" part of the word is not processed by the computer. The above card is followed by cards which contain the frequencies (ω) of the vibrational degrees of freedom of the molecule in 25X, 1F8.2 format. The number of frequency cards should be indicated in the next to last position on the species identification card. The total number of vibrational degrees of freedom should not exceed 12. The total combined number of linear and nonlinear polyatomic data packets cannot exceed 75.

For the data packets for the electrons, H^+ ion, and He^{++} ion, no energy level block is required.

B. Case Data

The case-data deck communicates to the computer both control data and thermodynamic condition data. The control data are used to inform the computer as to which "problem case" is to be considered and when "new data" are to be read into the machine. The "new data" may be either a change of initial pressure, initial temperature, initial mole fraction composition, or a complete change of the problem case and initial mixture constituents. Proper use of the control data will allow the user to run any combination of problem cases while varying the initial thermodynamic state and chemical composition at will.

The arrangement of the case data cards is summarized in Fig. 8. The format for the case data deck will be illustrated by the three following examples.

Example 1. Determine the thermodynamic properties for densities (ρ/ρ_A) of 0.1 and 0.01 and temperatures between 3000 and 7000°K. The symbol ρ_A is the density of air at standard conditions.

Example 2. Determine the thermodynamic properties and velocities associated with a normal shock in an initial mixture composed of 30% CO_2 and 70% N_2. The initial temperature is 300°K, and the initial pressure is 0.004 atm. The temperatures in the shock-heated gas are 4500°K, 5000°K, 5500°K, and 6000°K. Also, at the same final temperatures as listed above, consider the properties of shocks in a mixture of 50% CO_2 and 50% N_2, with an initial temperature of 300°K and an initial pressure of 0.004 atm.

Example 3. Determine the properties of both reflected and standing shocks resulting from traveling incident shocks in an air-like mixture composed of 78.08% N_2, 20.95% O_2, and 0.97% A. The initial temperature of the gaseous mixture is 300°K. The initial pressures considered are 0.001 and 0.01 atm. The temperatures behind the incident shock range from 4000 to 8000°K.

The form of case data for these examples is given in Tables 3, 4, and 5. The explanation of the format of the cards follows.

1. First Card

The first card of the case data deck supplies the total number of chemical species (compounds, ions, atoms, and the electron) and the total number of chemical elements (including the electron as a chemical element) which comprise the high temperature chemical equilibrium mixture. The information on this card is in format 2I2. The first word is the total number of elements in the mixture. The second word is the total number of chemical species.

In Example 1, the possible constituents of the high temperature mixture are N_2, N^{+++}, N^{++}, N^+, N_2^+, N, and e^-. The seven chemical species are composed of chemical elements N and e^-. Thus, the first word is 02, and the second is 07.

In Example 2, the chemical species are all those combinations of C, N, O, and e^- which are listed in Table 2. There are 32 of these. The number of elements plus electrons is 04.

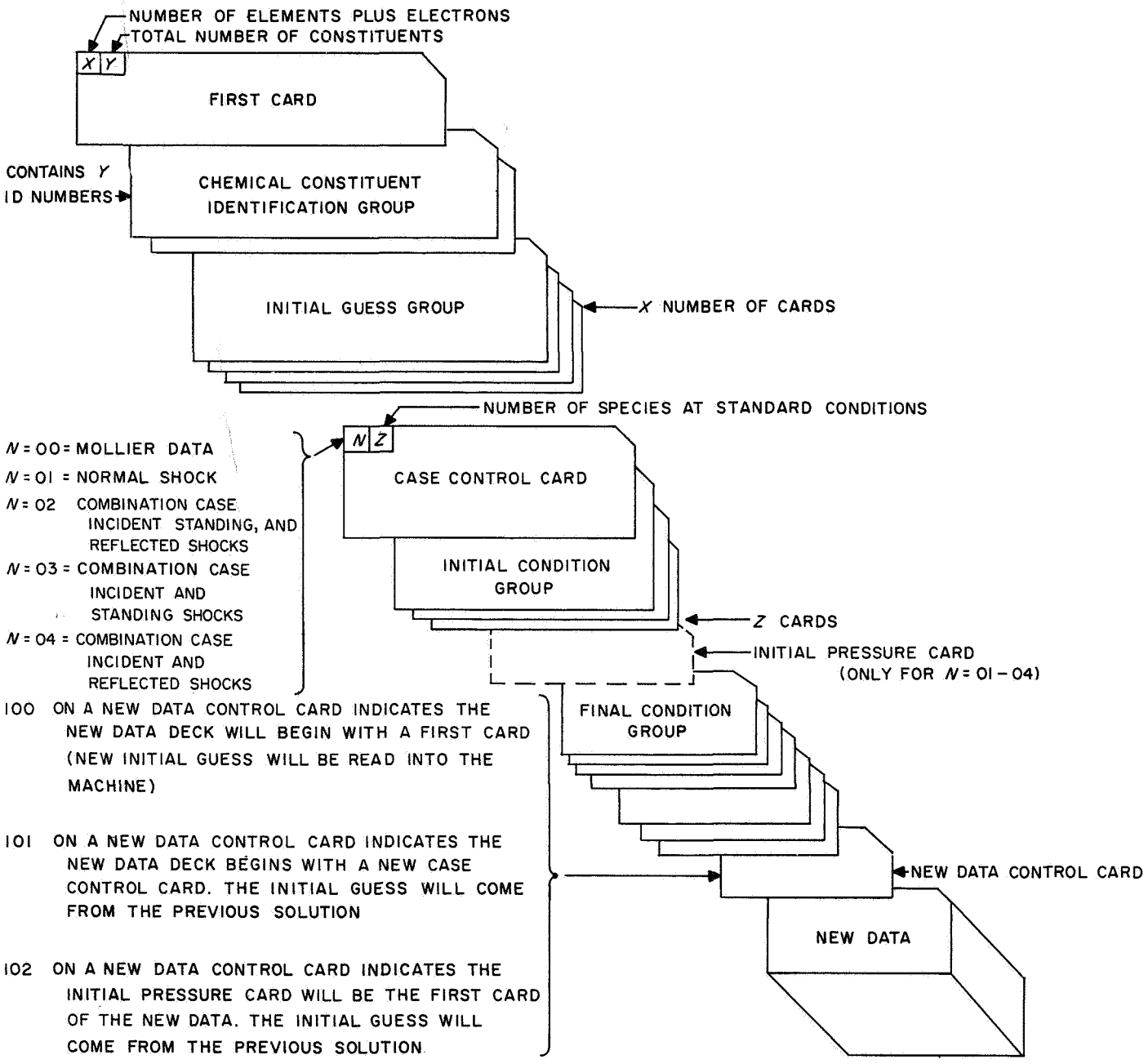


Fig. 8. The case data deck

Table 3. Example 1: Mollier data case

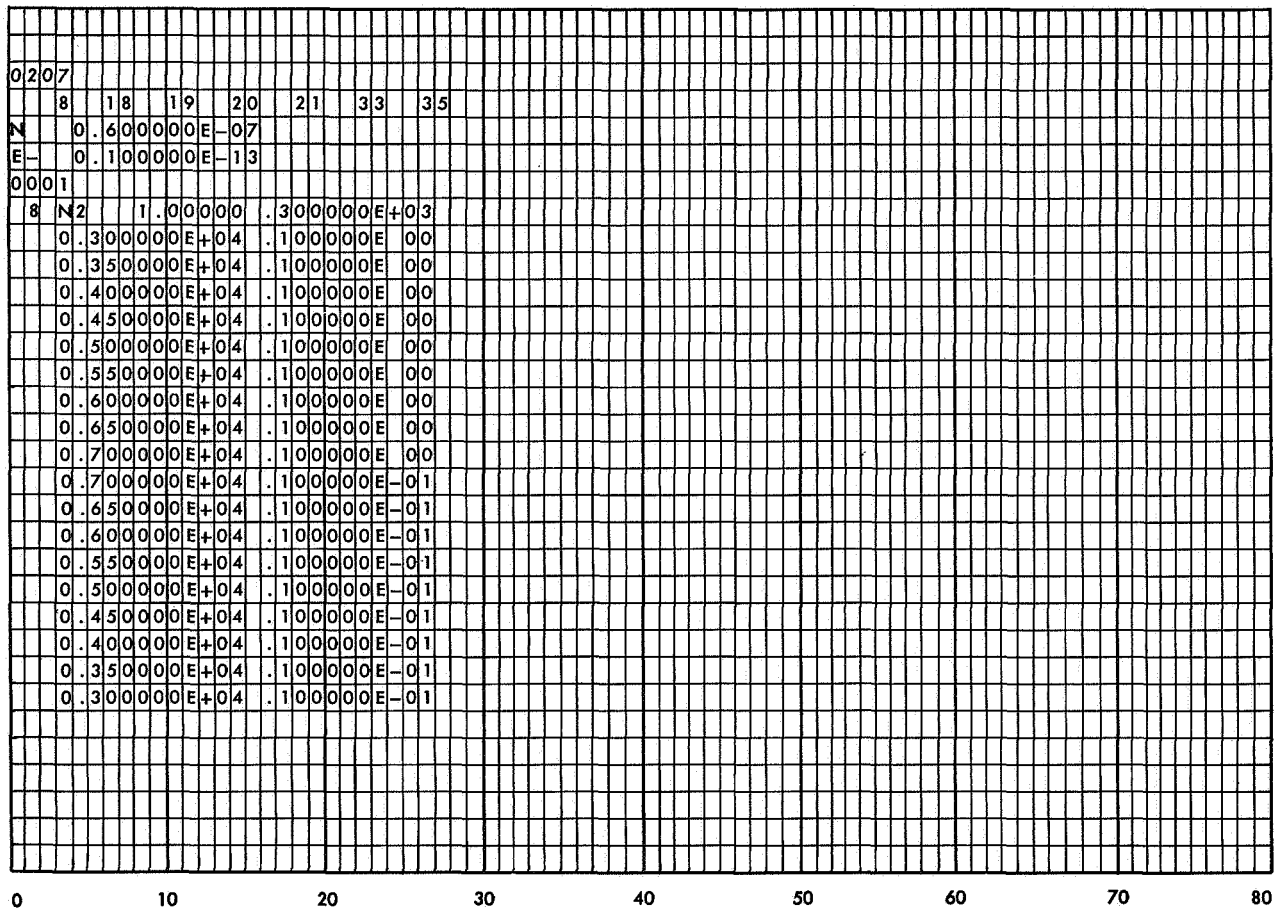
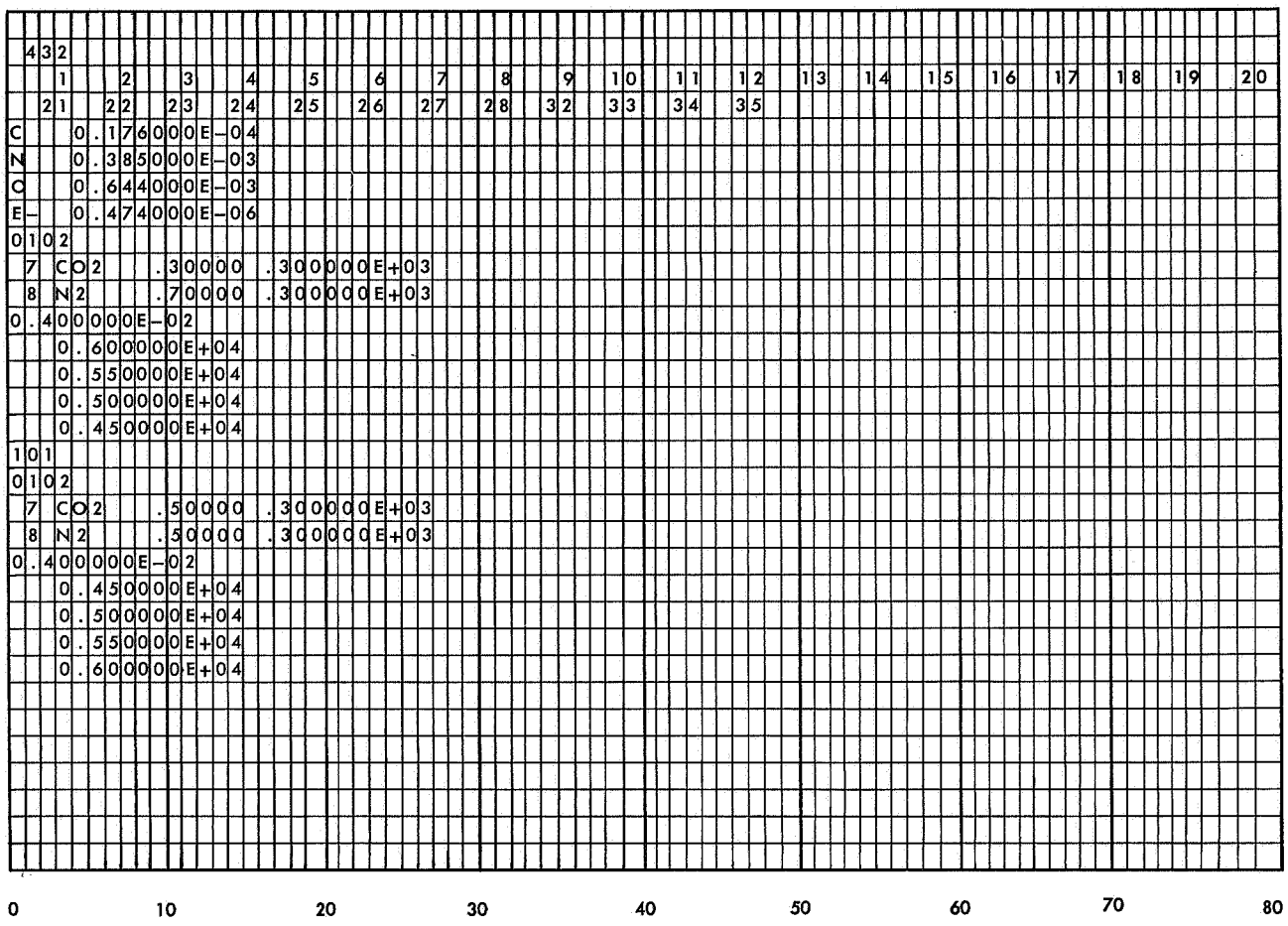


Table 4. Example 2: Moving normal shock case (30% CO_2 — 70% N_2 and 50% CO_2 — 50% N_2)



In Example 3, the constituent species are the combinations of N, O, e^-, and A which are listed in Table 2. There are 24 species which contain these four chemical elements.

2. *Chemical Constituent Identification Group*

This group consists of up to two cards which list the identification numbers of the constituent chemical species of the high temperature mixture. The identification numbers are found in Table 2. Each number is listed with an I4 format. With this format, there are a maximum of 20 identification numbers on each card. The identification numbers should be in order so that the chemical elements occur in the last positions. The number of identification numbers must equal the number in the second word position of the "first card."

For Example 1, the 7 constituents N_2, N^{+++}, N^{++}, N^+, N_2^+, N, and e^- have the identification numbers 8, 18, 19, 20, 21, 33, and 35, respectively. The seven values can be listed on one card. Two cards are required to list the 32 constituent identification numbers for Example 2 and two are required for identification numbers for Example 3.

3. *Initial Guess Cards*

There is an initial concentration guess card for each chemical element in the mixture. The number of initial guess cards is equal to the number appearing in the first word position of the "first card." The format for an initial guess card is 4X, 1E12.6. The first word position contains the chemical symbol for the element. The second word position contains the approximate concentration (mole/l) of the element at the first equilibrium state for which a solution is sought. The order of the initial guess cards should be the same as the order of the elements in Table 2.

As the convergence of numerical procedure for the chemical equilibrium computation is dependent upon the knowledge of a set of concentrations which nearly satisfy

Table 5. Example 3: Combination normal shock case (air mixture)

```
 424
    2    4    5    6    8    9   18   19   20   21   22   23   24   25   26   27   28   29   30   31
  33   34   35   36
N     0.180000E-05
O     0.160000E-03
E-    0.300000E-08
A     0.420000E-05
0203
 8 N2     0.78080  .300000E+03
 9 O2     0.20950  .300000E+03
36 A      0.00970  .300000E+03
1.000000E-03
    4.000000E+03
    4.500000E+03
    5.000000E+03
    5.500000E+03
    6.000000E+03
    6.500000E+03
    7.000000E+03
    7.500000E+03
    8.000000E+03
102
1.000000E-02
    8.000000E+03
    7.500000E+03
    7.000000E+03
    6.500000E+03
    6.000000E+03
    5.500000E+03
    5.000000E+03
    4.500000E+03
    4.000000E+03
```

0 10 20 30 40 50 60 70 80

the mass action and mass balance equations, the initial guess values are very important. If the initial guess values are in error by more than an order of magnitude, the convergence of the chemical equilibrium calculation is doubtful. The procedure for selecting the initial guesses is somewhat of an art which develops with the use of the program.

The program automatically uses the concentrations from the previous equilibrium calculation as the initial guess values for the next chemical equilibrium computation. Thus, the set of final and initial condition states should be arranged in an orderly progression to ensure convergence of the numerical procedure.

In the case of Example 1, the concentrations of 6×10^{-8} mole/l for N and 1×10^{-14} mole/l for the electrons are the approximate concentrations at a temperature of 3000°K and a density of 0.129 g/l. For Example 2, the concentrations (in mole/l) of

C	1.76×10^{-5}
N	3.85×10^{-4}
O	6.44×10^{-4}
e^-	4.74×10^{-7}

are associated with the temperature of 6000°K and the density of about 0.05 g/l. For Example 3, the concentrations of

N	1.8×10^{-6}
O	1.6×10^{-4}
e^-	3.0×10^{-9}
A	4.2×10^{-6}

are for a temperature of 4000°K and a density of about 0.01 g/l.

4. *Case Control Card*

The case control card contains two numbers in I2 format. The first number identifies the case of the problem to be considered. If this number is 00, the indication is that Mollier data is to be generated. If this number is 01, moving normal shock problems are to be solved. The number 03 indicates a combination case is desired consisting of an incident shock solution and a standing shock solution. For the number 04, one obtains a combination case in which incident shock and reflected shock properties are the result. With the number 02, a combination case consisting of incident, standing, and reflected shock conditions results. No other values are valid for the first word position on the case control card.

The second number on the card identifies the number of compounds present in the mixture at standard conditions. This number must equal the number of cards in the initial condition group.

5. *Initial Condition Group*

The format for the initial condition control card is I2, A6, 1F7.5, 1E12.6. There is one card for each of the initial constituents of the mixture. The number of cards in this group must be equal to the number in the second word position of the control card.

The first word is the species identification number taken from Table 2. The second word is the chemical symbol for the species. The third word is the mole-fraction of the species in the mixture at standard conditions. For the Mollier data case, this is all the information required on an initial condition group card, and any information in the fourth position is read into the computer but is not utilized in the computations.

For the moving and combination normal shock cases, the value in the fourth word position is the initial temperature, T_1.

The order of the cards within the initial condition group is not important; however, the best procedure would be to arrange the identification numbers which appear on them in order. The data on these cards are not only used to calculate the thermodynamic properties of the gas at standard and initial conditions, but also are used with the library data to calculate the values of B_i which appear in the mass action equations.

For Example 1, the 100% N_2-Mollier data case, there is only one card in the initial condition group. The first word is 08 (which agrees with the specie identification number for N_2 in Table 2). The position and format of the chemical formula and mole-fraction are shown in Table 3. Normally, the fourth position would be vacant for a Mollier data case. The value listed for the temperature will not effect the operation of the program as it is not used in Mollier data computations.

For Example 2, the first card of the initial condition group corresponds to CO_2 and contains the specie ID number of 07, the mole-fractional concentration at standard conditions of 0.3, and the initial temperature of 300°K. The second card corresponds to the compound N_2 and contains the ID number of 08, the mole-fraction of 0.7, and the initial temperature of 300°K.

For Example 3, the cards list:

ID No.	Chemical symbol	Mole-fraction @ STP	Initial temperature, °K
08	N_2	0.7808	300
09	O_2	0.2095	300
36	A	0.0097	300

6. *Initial Pressure Card*

The initial pressure card is not included when the Mollier data case is to be run. The card contains the pressure of the gas in atmospheres before the passage of the shock. The pressure value is in a format E12.6.

In Example 1, the initial pressure card is not necessary.

In Example 2, the initial pressure is 0.04 atm. Farther down in the new case data, the initial pressure of 0.04 atm is repeated for the 50%-CO_2 and 50%-N_2 mixture.

In Example 3, the first initial pressure is 0.001 atm. In the new data, the initial pressure is changed to 0.01 atm.

7. *Final Condition Group*

The final condition group is composed of an unlimited number of cards. There is one card for each thermodynamic or shock condition. The thermodynamic condition associated with the first card of this group should be compatible with the concentrations listed on the initial guess cards.

For the Mollier data cases, each card specifies the temperature and density of the thermodynamic state for which the chemical equilibrium composition and properties are to be calculated. The format for a Mollier data case, final condition group card is 3X, 2E12.6. The first three spaces are blank, followed by the first word which is the temperature in °K. The second word is the ratio of density at the solution point to density of air at standard conditions. Experience has shown that the most efficient way of calculating data over a range of temperatures and densities is to calculate a series of temperatures while holding the density constant, then change the density by not more than an order of magnitude and calculate through the series of temperatures in reverse order, and so on.

For the shock cases, the format of the final condition cards is 3X, 1E12.6. The first three spaces are left blank, followed by the temperature in °K. The first card of a final condition group should correspond to the concentrations listed on the initial guess cards. The temperatures listed on the final condition group cards are not limited in any way.

8. New Data Control Card

A new data control card is used for the following options:

(1) To change initial pressure in normal shock and combined shock cases.

(2) To change initial mixture mole-fractions and/or to change initial temperature and/or change cases.

(3) To completely change the problem by reading in a completely new deck of case data beginning with the "first card."

If the computations are complete when the last card of the final condition group has been processed, then the new data card is not used. However, if as shown in Table 5, an option such as (1) is considered, with the initial pressure changed from 10^{-3} to 10^{-2} atm, then a new data card with 102 must be used to preface the new data. In this option, the new data consists of a new pressure card followed by a new final condition group. Note that the last temperature and first temperature of the new data are the same to ensure convergence at the new pressure.

If an option such as (2) is desired, the new data control card should contain a 101. This will cause the machine to read in a new set of data which should consist of new case control card, initial condition group, initial pressure card, and final condition group. An example illustrating the use of the 101 new data control card is given in Table 4, where the card is used to change the mole-fraction composition of the CO_2-N_2 mixture for a moving normal shock case. Because the program uses the concentrations from the previous calculation as the initial guesses for the new calculations, the change in initial state and concentration should not be large.

The option (3) is achieved by using the 100 new data control card. After this card, a completely new set of case data, beginning with "first card," should follow. A 100 new data control card used between each of the example data of Tables 3, 4, and 5 would allow the three problems to be solved in succession.

VII. Program Output

The output for the first solution of each of the three example cases is shown in Tables 6, 7, and 8.

Table 6. Chemical equilibrium composition and properties of a complex mixture

```
INITIAL CONDITIONS
                    MOLE FRACTION OF  N2    AT S.T.P.---1.00000
FINAL CONDITIONS
             CONCENTRATION       MOLE FRACTION
          PARTICLES/CC  MOLE/LITER
N2        0.2779E 19  0.4613E-02  1.0000E 00
N+++      0.6023E-14  1.0000E-35  0.2168E-32
N++       0.6023E-14  1.0000E-35  0.2168E-32
N+        0.4229E 04  0.7020E-17  0.1522E-14
N2+       0.5718E 07  0.9492E-14  0.2058E-11
N         0.3611E 14  0.5996E-07  0.1300E-04
E-        0.5722E 07  0.9500E-14  0.2059E-11
TEMPERATURE (DEG K)----- 0.3000E 04  P/P0--------0.1136E 01  ENTROPY (SM0/R)---------0.3196E 02
ENTHALPY (HM0/RT0)------ 0.4463E 02  RHO/RH00----0.1000E-00  RH00--------------------0.1292E 01
MIXTURE COLD MOL WT----- 0.2801E 02  Z-----------0.1000E 01
```

Table 7. Real gas normal shock-wave properties

```
 INITIAL CONDITIONS
TEMPERATURE (DEG K)----- 0.3000E 03  RHO1/RHO0---0.4126E-02  RHO0 (GM/LITER)---------0.1292E 01
ENTHALPY (HMO/RTO)-------0.4799E 02  P1/P0-------0.4000E-02  MIXTURE COLD MOL WT-----0.3281E 02
                     MOLE FRACTION OF  CO2    AT S.T.P.---0.30000
                     MOLE FRACTION OF  N2     AT S.T.P.---0.70000
 FINAL CONDITIONS
             CONCENTRATION       MOLE FRACTION
         PARTICLES/CC  MOLE/LITER
 CN      0.1363E 16  0.2264E-05  0.7475E-03
 NO+     0.2582E 15  0.4286E-06  0.1416E-03
 CO      0.3807E 18  0.6321E-03  0.2087E-00
 NO      0.1149E 17  0.1908E-04  0.6300E-02
 NO2     0.6960E 11  0.1155E-09  0.3816E-07
 N2O     0.6417E 12  0.1065E-08  0.3518E-06
 CO2     0.7981E 14  0.1325E-06  0.4376E-04
 N2      0.7937E 18  0.1318E-02  0.4351E-00
 O2      0.3218E 15  0.5343E-06  0.1764E-03
 C+++    0.6023E-14  1.0000E-35  0.3302E-32
 C++     0.7776E-01  0.1291E-21  0.4263E-19
 C+      0.1807E 14  0.3000E-07  0.9908E-05
 C-      0.5384E 10  0.8938E-11  0.2952E-08
 CO+     0.9704E 13  0.1611E-07  0.5320E-05
 C2N2    0.4430E 10  0.7355E-11  0.2429E-08
 C2      0.4501E 13  0.7473E-08  0.2468E-05
 C3      0.1058E 10  0.1756E-11  0.5800E-09
 N+++    0.6023E-14  1.0000E-35  0.3302E-32
 N++     0.1648E-05  0.2736E-26  0.9035E-24
 N+      0.2420E 13  0.4017E-08  0.1326E-05
 N2+     0.1344E 13  0.2231E-08  0.7366E-06
 O+++    0.6023E-14  1.0000E-35  0.3302E-32
 O++     0.2608E-09  0.4330E-30  0.1430E-27
 O+      0.4931E 13  0.8187E-08  0.2704E-05
 O-      0.5673E 12  0.9419E-09  0.3110E-06
 O2-     0.2388E 09  0.3964E-12  0.1309E-09
 O2+     0.1584E 12  0.2630E-09  0.8685E-07
 O3      0.8013E 08  0.1330E-12  0.4393E-10
 C       0.1062E 17  0.1763E-04  0.5821E-02
 N       0.2327E 18  0.3864E-03  0.1276E-00
 O       0.3924E 18  0.6514E-03  0.2151E-00
 E-      0.2942E 15  0.4885E-06  0.1613E-03
SHOCK VELOCITY (FPS)---- 0.1813E 05  RHO2/RHO0-- 0.5520E-01  VEL BEHIND SHOCK (FPS)--0.1678E 05
TEMPERATURE (DEG K)----- 0.6000E 04  RHO2/RHO1-- 0.1338E 02  ENTROPY (SMO/R)---------0.4649E 02
ENTHALPY (HMO/RTO)------ 0.1714E 03  P2/P0------ 0.1491E 01  Z-----------------------0.1393E 01
STAG ENTHALPY (HMO/RTO)- 0.1726E 03  P2/P1------ 0.3727E 03
```

For a Mollier data case, the format is shown in Table 6. Listed are the initial conditions, where the composition of the mixture at standard temperature and pressure is given. The chemical concentration of each specie in the heated mixture is listed under "Final Conditions." The first column is the concentration in particles per cubic centimeter, and the second column is in mole per liter. The third column lists the mole fraction concentration.

The tabulation of specie concentration is followed by a display of the thermodynamic properties in dimensionless form. These values are; the temperature in °K; the dimensionless enthalpy per unit mass (HM_o/RT_o); the cold mixture molecular weight; the pressure in atmospheres ($P_o = 1$ atm); the dimensionless density; Z as defined in Eq. (19); the entropy in dimensionless form (SM_o/R); and $RHO0 = \rho_0$, which is the density of air in g/l at standard conditions. The R is the universal gas constant 1.98726 cal/mole-°K; M_o is the cold molecular weight, and T_o is 273.15°K.

The forms of the output data for the moving normal shock case and the combination normal shock case are shown in Tables 7 and 8. The two are similar except for the additional listings in Table 8 of the properties of the standing and reflected normal shocks. For the combination cases 03 and 04, the output consists of listings of the moving and standing shocks, and moving and reflected shocks, respectively. The description of the concentration and thermodynamic property display given

Table 8. Combination normal shock solutions

```
    (6)  REAL GAS NORMAL SHOCK WAVE PROPERTIES
 INITIAL CONDITIONS
TEMPERATURE (DEG K)----- 0.3000E 03  RHO1/RHO0---0.9104E-03  RHO0 (GM/LITER)---------0.1292E 01
ENTHALPY (HMO/RTO)------ 0.3835E 01  P1/P0-------1.0000E-03  MIXTURE COLD MOL WT-----0.2896E 02
                      MOLE FRACTION OF  N2     AT S.T.P.---0.78080
                      MOLE FRACTION OF  02     AT S.T.P.---0.20950
                      MOLE FRACTION OF  A      AT S.T.P.---0.00970
 FINAL CONDITIONS
             CONCENTRATION       MOLE FRACTION
         PARTICLES/CC  MOLE/LITER
 NO+     0.1784E 13  0.2962E-08  0.5675E-05
 NO      0.6641E 16  0.1102E-04  0.2112E-01
 NO2     0.1607E 12  0.2669E-09  0.5113E-06
 N20     0.1345E 12  0.2233E-09  0.4277E-06
 N2      0.2025E 18  0.3361E-03  0.6440E 00
 02      0.2431E 16  0.4037E-05  0.7734E-02
 N+++    0.6023E-14  1.0000E-35  0.1916E-31
 N++     0.6023E-14  1.0000E-35  0.1916E-31
 N+      0.7968E 06  0.1323E-14  0.2534E-11
 N2+     0.7639E 07  0.1268E-13  0.2430E-10
 O+++    0.6023E-14  1.0000E-35  0.1916E-31
 O++     0.6023E-14  1.0000E-35  0.1916E-31
 O+      0.2184E 09  0.3626E-12  0.6947E-09
 O-      0.6597E 10  0.1095E-10  0.2099E-07
 O2-     0.3635E 08  0.6035E-13  0.1156E-09
 02+     0.9947E 09  0.1651E-11  0.3164E-08
 03      0.3434E 09  0.5702E-12  0.1092E-08
 AR+++   0.6023E-14  1.0000E-35  0.1916E-31
 AR++    0.6023E-14  1.0000E-35  0.1916E-31
 AR+     0.1289E 06  0.2141E-15  0.4101E-12
 N       0.1075E 16  0.1785E-05  0.3421E-02
 O       0.9921E 15  0.1647E-03  0.3156E-00
 E-      0.1779E 13  0.2953E-08  0.5657E-05
 AR      0.2563E 16  0.4255E-05  0.8153E-02
SHOCK VELOCITY (FPS)---- 0.1319E 05  RHO2/RHO0-- 0.9832E-02  VEL BEHIND SHOCK (FPS)--0.1197E 05
TEMPERATURE (DEG K)----- 0.4000E 04  RHO2/RHO1-- 0.1080E 02  ENTROPY (SMO/R)----------0.3997E 02
ENTHALPY (HMO/RTO)------ 0.1060E 03  P2/P0------ 0.1713E-00  Z-------------------------0.1190E 01
STAG ENTHALPY (HMO/RTO)- 0.1069E 03  P2/P1------ 0.1713E 03
```

above for the Mollier data case is applicable to the shock solution cases. Under the heading "Initial Conditions" are the temperature, dimensionless enthalpy, density and pressure, mixture molecular weight, and composition of the initial unshocked gas. The heading "Final Conditions" is equivalent to subscripting the properties with 2 for the moving shock, 3 for the standing shock, and 4 for the reflected shock.

The quantities listed below the concentrations of the moving normal shock are: velocity, U_s, or free-flight velocity, U_f, in ft/sec; temperature, T_2; dimensionless enthalpy, $H_2 M_o/RT_o$; dimensionless stagnation enthalpy on a free-flight body; the density ratios ρ_2/ρ_o and ρ_2/ρ_1; pressure ratios P_2/P_o and P_2/P_1; the velocity U_g associated with the moving normal shock; the entropy, $S_2 M_o/R$; and $Z_2 = M_o/M_2$.

The final conditions listed under the heading "Real Gas Standing Normal Shock Wave Properties" are: the concentrations behind the standing wave; the moving shock velocity; temperature, T_3; dimensionless enthalpy, $H_3 M_o/RT_o$; "cold" molecular weight, M_o; pressure, P_3, in atmospheres; pressure ratio, P_3/P_2; density ratios ρ_3/ρ_o and ρ_3/ρ_2; standard density, ρ_o; velocity behind the standing shock, U_3, in ft/sec; dimensionless stagnation enthalpy on the model; dimensionless entropy, $S_3 M_o/R$; and Z_3.

The final conditions listed under the heading "Real Gas Reflected Normal Shock Wave Properties" are: the concentrations behind the reflected wave; the shock velocity, U_s; temperature, T_4; dimensionless enthalpy, $H_4 M_o/RT_o$; "cold" molecular weight, M_o; the pressure, P_4, in atmospheres; the pressure ratio, P_4/P_2; the density ratios, ρ_4/ρ_o and ρ_4/ρ_2; the reflected shock velocity in ft/sec; dimensionless entropy, $S_4 M_o/R$; Z_4 and ρ_o.

The program prints one shock solution per page. For the combination case shown in Table 8, the solutions for

Table 8 (contd)

```
    (b) REAL GAS STANDING NORMAL SHOCK WAVE PROPERTIES
INITIAL CONDITIONS  TEMP DEG K--0.3000E 03       P/P0--1.0000E-03
                    MOLE FRACTION OF  N2    AT S.T.P.---0.78080
                    MOLE FRACTION OF  02    AT S.T.P.---0.20950
                    MOLE FRACTION OF  A     AT S.T.P.---0.00970
 FINAL CONDITIONS
            CONCENTRATION       MOLE FRACTION
         PARTICLES/CC  MOLE/LITER
 NO+     0.3763E 15  0.6248E-06  0.2038E-03
 NO      0.1787E 17  0.2967E-04  0.9678E-02
 NO2     0.1494E 12  0.2480E-09  0.8090E-07
 N2O     0.1106E 13  0.1836E-08  0.5988E-06
 N2      0.9560E 18  0.1587E-02  0.5177E 00
 02      0.6224E 15  0.1033E-05  0.3370E-03
 N+++    0.6023E-14  1.0000E-35  0.3262E-32
 N++     0.6023E-14  1.0000E-35  0.3262E-32
 N+      0.3084E 13  0.5120E-08  0.1670E-05
 N2+     0.1744E 13  0.2895E-08  0.9442E-06
 O+++    0.6023E-14  1.0000E-35  0.3262E-32
 O++     0.6023E-14  1.0000E-35  0.3262E-32
 O+      0.7421E 13  0.1232E-07  0.4019E-05
 O-      0.1044E 13  0.1733E-08  0.5652E-06
 O2-     0.5906E 09  0.9806E-12  0.3199E-09
 O2+     0.3041E 12  0.5049E-09  0.1647E-06
 O3      0.2230E 09  0.3702E-12  0.1208E-09
 AR+++   0.6023E-14  1.0000E-35  0.3262E-32
 AR++    0.6023E-14  1.0000E-35  0.3262E-32
 AR+     0.3573E 11  0.5932E-10  0.1935E-07
 N       0.2831E 18  0.4700E-03  0.1533E-00
 O       0.5744E 18  0.9536E-03  0.3111E-00
 E-      0.3879E 15  0.6440E-06  0.2101E-03
 AR      0.1375E 17  0.2282E-04  0.7446E-02
SHOCK VELOCITY (FPS)---- 0.1319E 05  P3/P0--------0.1526E 01  VEL BEHIND ST SHOCK-----0.2231E 04
TEMPERATURE (DEG K)----- 0.6066E 04  P3/P2--------0.8907E 01  STAG ENTHALPY (HM0/RT0)-0.1900E 03
ENTHALPY (HM0/RT0)------ 0.1870E 03  RH03/RH00---0.5275E-01  ENTROPY (SM0/R)---------0.4157E 02
M0-MIXTURE COLD MOL WT-- 0.2896E 02  RH03/RH02---0.5364E 01  Z ----------------------0.1303E 01
                                     RH00 (GM/L)-0.1292E 01
```

the moving, standing and reflected shocks were printed on three pages. To prevent the shock solution of a complicated mixture, involving many species, from listing the output on more than one page, the program will list the specie concentrations in two columns when the number of species is larger than 35. An example of this is shown in the moving shock solution of Table 9. This solution is for a mixture of 94% air and 6% water vapor at an initial pressure of 1 mm Hg (0.00131579 atm) and a final temperature of 10,000°K. Since the number of species is larger than 35, the concentrations are listed in two sets.

In addition to the above "scheduled" output, the program has been designed to halt all computations when the number of iteration loops through the equilibrium block exceeds 50, or when the number of iteration loops through the moving normal shock equations exceeds 20. After 50 equilibrium block iterations, the program prints "equilibrium state not reached in 50 iterations" followed by a tabulation of the concentrations for the last two iterations. After 20 normal shock iterations, the machine prints "no Hugoniot solution in 20 iterations" and halts.

VIII. Discussion

The accuracy of the program has been checked in a number of ways. First, the accuracy of the matrix inversion portion of the program was checked and found to give correct solutions to arbitrary systems of 10 simultaneous linear equations accurate to seven figures. Second, through comparisons with hand computations the accuracy of the equilibrium solutions have been proven. The basic convergence criteria has been shown to be reliable by the comparison of successive interactions. Perhaps one should realize that the concentrations of electrons and ions can be in error at low temperature, below 2000°K or 3000°K, due to the fact that when such a small concentration is present, a change in their concentration results in a negligible change in gross properties. In every case encountered in four years of

Table 8 (contd)

```
    (c)  REAL GAS REFLECTED NORMAL SHOCK WAVE PROPERTIES
INITIAL CONDITIONS  TEMP DEG K--0.3000E 03       P/P0--1.0000E-03
                    MOLE FRACTION OF  N2     AT S.T.P.---0.78080
                    MOLE FRACTION OF  O2     AT S.T.P.---0.20950
                    MOLE FRACTION OF  A      AT S.T.P.---0.00970
 FINAL CONDITIONS
              CONCENTRATION       MOLE FRACTION
         PARTICLES/CC  MOLE/LITER
 NO+     0.7230E 15  0.1200E-05  0.3002E-03
 NO      0.1982E 17  0.3290E-04  0.8227E-02
 NO2     0.1473E 12  0.2445E-09  0.6115E-07
 N2O     0.1391E 13  0.2309E-08  0.5774E-06
 N2      0.1095E 19  0.1818E-02  0.4545E-00
 O2      0.5366E 15  0.8908E-06  0.2228E-03
 N+++    0.6023E-14  1.0000E-35  0.2501E-32
 N++     0.6023E-14  1.0000E-35  0.2501E-32
 N+      0.2012E 14  0.3340E-07  0.8354E-05
 N2+     0.7846E 13  0.1303E-07  0.3258E-05
 O+++    0.6023E-14  1.0000E-35  0.2501E-32
 O++     0.6023E-14  1.0000E-35  0.2501E-32
 O+      0.2772E 14  0.4601E-07  0.1151E-04
 O-      0.1972E 13  0.3274E-08  0.8189E-06
 O2-     0.8511E 09  0.1413E-11  0.3534E-09
 O2+     0.6363E 12  0.1056E-08  0.2642E-06
 O3      0.2182E 09  0.3623E-12  0.9061E-10
 AR+++   0.6023E-14  1.0000E-35  0.2501E-32
 AR++    0.6023E-14  1.0000E-35  0.2501E-32
 AR+     0.1748E 12  0.2903E-09  0.7259E-07
 N       0.5545E 18  0.9206E-03  0.2302E-00
 O       0.7202E 18  0.1196E-02  0.2990E-00
 E-      0.7775E 15  0.1291E-05  0.3228E-03
 AR      0.1717E 17  0.2851E-04  0.7130E-02
SHOCK VELOCITY (FPS)---- 0.1319E 05  P4/P0-------0.2128E 01  REF SHOCK VEL (FPS)-----0.2100E 04
TEMPERATURE (DEG K)----- 0.6487E 04  P4/P2-------0.1242E 02  ENTROPY (SM0/R)---------0.4255E 02
ENTHALPY (HM0/RT0)------ 0.2196E 03  RH04/RH00---0.6589E-01  Z-----------------------0.1360E 01
M0-MIXTURE COLD MOL WT-- 0.2896E 02  RH04/RH02---0.6700E 01  RH00--------------------0.1292E 01
```

experience with the JPL Thermochemistry and Normal Shock Program where errors were encountered, they are in species of negligible concentration. Mostly, this is because, in any machine computation, we reach a point where the numbers computed are either so small or large that they exceed the capacity of the computer. In some cases as in this program, it is not advisable to call these small quantities zero. To alleviate this difficulty in our equilibrium computations, we have considered all concentrations less than 10^{-35} moles/liter, which corresponds to approximately 6×10^{-15} particles/cm^3 to be equal to 10^{-35} moles/liter. Concentrations of this magnitude are obviously negligible, but are included in the output.

Finally the accuracy of the shock solutions have been proven by spot comparison with a variety of shock parameter tabulations including Refs. 12, 30, and 45. Also, the results of the present program have been compared with those of its predecessor. In all cases where comparable thermochemistry was used, the shock parameter and concentrations were in agreement to 3 or 4 figures. As some of these computations were performed using only 4 significant figures, this agreement would seem remarkable. However, comparison of the result of the program computed, using 4 significant figures with those using 8 figures, reveals agreement for concentrations to 3 to 4 figures; thus, the round off errors are not severe when using only 4 significant figures in the computations.

In computing properties of a variety of mixtures over a wide range of conditions, not a single case has been encountered in which the program has failed to achieve a solution. All failures of the program to converge to a solution or to yield obviously erroneous results have been associated with the failure of the user to exercise proper care in treating the input data.

A word of caution about using the program in extreme ranges of temperature and pressure is called for at this point. As has been pointed out intentionally in the comments on the literature given in the Appendix A, caution must be used at a low temperature when the pressure

Table 9. Moving normal shock solution for an air-water vapor mixture

```
        REAL GAS NORMAL SHOCK WAVE PROPERTIES
 INITIAL CONDITIONS
TEMPERATURE (DEG K)----- 0.3000E 03  RHO1/RHO0---0.1171E-02  RHO0 (GM/LITER)---------0.1292E 01
ENTHALPY (HM0/RT0)-------0.2443E 01  P1/P0-------0.1316E-02  MIXTURE COLD MOL WT-----0.2831E 02
                     MOLE FRACTION OF  N2    AT S.T.P.---0.73400
                     MOLE FRACTION OF  02    AT S.T.P.---0.19700
                     MOLE FRACTION OF  H20   AT S.T.P.---0.06000
                     MOLE FRACTION OF  AR    AT S.T.P.---0.00900
 FINAL CONDITIONS
            CONCENTRATION      MOLE FRACTION              CONCENTRATION      MOLE FRACTION
        PARTICLES/CC  MOLE/LITER                      PARTICLES/CC  MOLE/LITER
 N2     0.3273E 16  0.5434E-05  0.3267E-02   02      0.2417E 13  0.4013E-08  0.2413E-05
 H2     0.3756E 12  0.6235E-09  0.3749E-06   NO      0.1253E 15  0.2079E-06  0.1250E-03
 NH     0.8646E 13  0.1435E-07  0.8629E-05   OH      0.2753E 13  0.4570E-08  0.2748E-05
 N2+    0.3881E 14  0.6443E-07  0.3873E-04   NO-     0.8265E 09  0.1372E-11  0.8249E-09
 NO+    0.1113E 15  0.1848E-06  0.1111E-03   02+     0.3786E 12  0.6285E-09  0.3778E-06
 02-    0.3358E 08  0.5575E-13  0.3352E-10   OH+     0.1493E 12  0.2479E-09  0.1490E-06
 OH-    0.2338E 08  0.3881E-13  0.2333E-10   H2+     0.1394E 11  0.2315E-10  0.1391E-07
 N20    0.7034E 09  0.1168E-11  0.7021E-09   N02     0.5101E 08  0.8469E-13  0.5092E-10
 NH3    0.3053E 02  0.5068E-19  0.3047E-16   03      0.1793E 06  0.2976E-15  0.1789E-12
 H20    0.8986E 07  0.1492E-13  0.8968E-11   N-      0.4738E 13  0.7867E-08  0.4729E-05
 N+     0.1568E 17  0.2603E-04  0.1565E-01   N++     0.2847E 07  0.4727E-14  0.2842E-11
 N+++   0.1435E-12  0.2382E-33  0.1432E-30   0-      0.3045E 13  0.5056E-08  0.3039E-05
 0+     0.3197E 16  0.5308E-05  0.3191E-02   0++     0.3320E 04  0.5513E-17  0.3314E-14
 0+++   0.6023E-14  1.0000E-35  0.6012E-32   H-      0.2798E 12  0.4645E-09  0.2793E-06
 H+     0.9660E 15  0.1604E-05  0.9641E-03   AR+     0.6625E 14  0.1100E-06  0.6612E-04
 AR++   0.3084E 06  0.5120E-15  0.3078E-12   AR+++   0.9068E-10  0.1505E-30  0.9051E-28
 N      0.6828E 18  0.1134E-02  0.6815E 00   0       0.2147E 18  0.3564E-03  0.2143E-00
 H      0.5668E 17  0.9410E-04  0.5657E-01   AR      0.4258E 16  0.7069E-05  0.4250E-02
 E-     0.2005E 17  0.3329E-04  0.2001E-01
SHOCK VELOCITY (FPS)---- 0.3246E 05  RHO2/RHO0-- 0.1747E-01  VEL BEHIND SHOCK (FPS)--0.3028E 05
TEMPERATURE (DEG K)----- 0.1000E 05  RHO2/RHO1-- 0.1492E 02  ENTROPY (SM0/R)---------0.5841E 02
ENTHALPY (HM0/RT0)------ 0.6048E 03  P2/P0------ 0.1365E 01  Z----------------------0.2085E 01
STAG ENTHALPY (HM0/RT0)- 0.6076E 03  P2/P1------ 0.1037E 04
```

is high, i.e., over 100 atm and at high temperature. There is a limited temperature-pressure range in which the ideal or perfect real-gas assumptions used in this program are valid. At low temperatures, the boundary is determined by the "van der Waals" forces which become important at high densities. At high pressure and temperature, the problem of computing gas properties depends upon the shift in ionization potential and energy levels due to the coulombic or Debye type of micro-field associated with a plasma. This problem of defining the range of application of the results of this program are discussed further in Ref. 38.

Appendix A

Review of Some of the Literature on Computation of Equilibrium Properties of Mixtures

(1966) Koopman (Ref. 2, 1966): An iterative procedure has been developed and programmed in MAD computer language for the calculation of the states attained behind incident and reflected shocks in fully dissociated and partially ionized gases. The calculations include the effects of truncation of the partition function sum and lowering of the ionization potential, effects which the author states "have only a modest effect on the determination of the final electron density under conditions encountered in shock tubes." The final equilibrium mixtures can include only atomic and ionic forms of neon, argon, hydrogen, oxygen, sulfur, carbon, and nitrogen.

(1966) Zelenik and Gordon (Ref. 3, 1966): An iterative method for calculating the equilibrium composition and thermodynamic properties of a mixture of atomic and ionic species is presented in which both the Debye-Hückel and the ionization potential lowering effects are considered.

(1965) Drellishak, Aeschliman, and Cambel (Ref. 4, 1965) (Ref. 14, 1963); Drellishak (Ref. 13, 1964): The physical problems in computing partition function and chemical composition of a gas mixture consisting of atoms, molecules, and ions, including the effect of the Debye cutoff criterion and lowering of the ionization potential are discussed. For the molecular species, different degrees of sophistication have been examined in computing ground-state rotational-vibrational contribution to the partition functions. Results in the form of chemical composition and internal partition functions of argon, nitrogen, and oxygen plasma are presented in graphical form up to 35,000°K for pressures between 0.01 and 5 atm.

(1965) Lewis and Burges (Ref. 5, 1965); Lewis and Neel (Ref. 10, 1964) (Ref. 12, 1964): A compilation of normal shock-wave parameters is presented, which is based upon the early imperfect real-gas thermodynamic properties of air computed by Hilsenrath and Klein. The altitude-velocity charts extend up to velocities of 50,000 fps and up to altitudes of 400,000 ft. The shock tables present incident, standing, and reflected shock parameters in air for incident shock Mach numbers up to 30. In a comparison of imperfect and perfect specific heats and speeds of sound, the differences were found to be "modest" for temperatures below 15,000°K and pressures below 100 atm.

(1965) Hilsenrath and Klein (Ref. 6, 1965): An extensive tabulation is presented of thermodynamic properties and chemical composition (28 species) of air from 1500°K to 15,000°K in 100°K increments and at close density intervals. The effects of second virial corrections at high pressures and Debye-Hückel corrections at high electron concentrations were included. The appendix of this report contains an excellent review by A. R. Hochstim of early calculations of thermodynamic properties of air.

(1964) Hester and Sewell (Ref. 11, 1964); Sewell (Ref. 19, 1962); (Ref. 31, 1961); Fenter and Gibbons (Ref. 33, 1961): These studies are tabulations of chemical compositions and equilibrium properties of nitrogen, argon, air, and helium for a wide range of densities and temperatures up to 100,000°K. These data are based upon ideal or perfect real-gas analysis with the exception of helium, in which the influence of truncating the partition function sum at different principal quantum numbers was examined. In this case allowing n_{min} to vary and holding $n_{max} = 4$ fixed, this results in only 2% deviation in the thermodynamic properties.

(1964) McChesney and Jones (Ref. 7, 1964): The equilibrium shock parameters for xeon are calculated for initial pressures between 0.5 and 750 mm Hg and shocked gas temperatures up to 20,000°K. Also, the problem of determining the electronic partition function of the atomic and ionic species is discussed. By means of computed examples, the role of both the missing energy levels and the Debye-Hückel effects is examined. The authors' conclusion is that for the normal range of shock tube experiments, the differences arising from the Debye-Hückel theory and the missing energy levels do not seriously modify the properties of a shock ionized plasma. Because of its low ionization potentials, one would expect the effects of partition function truncation procedures, ionization potential lowering, and missing energy levels to be more pronounced in xeon than in the other noble gases.

(1964) Pinkus (Ref. 9, 1964): This investigation presented in tabular form for the properties of air at relatively low temperatures (subcritical to 1500°K) but at high pressures (up to 1000 atm) where real-gas phenomena are dominated by "van der Waals" type forces. The computations are based upon an equation of state proposed by Hirschfelder. Also, the plenum conditions for both isothermal and isentropic expansion conditions are given.

(1964) Kubin and Presley (Ref. 8, 1964): These authors have made computations on hydrogen based on the assumption of ideal mixture behavior with only 6 electronic states used in the electronic partition function evaluation, no lowering of the ionization potential, and treatment of molecular hydrogen as a rigid rotation-harmonic oscillation in its electronic ground state. The results are within a few percent of the "more rigorous" computations of Rosenbaum and Levitt.

(1963) Vasiliu (Ref. 15, 1963): This report presents tables of air properties at high pressures obtained from a computer program developed for this purpose. The approximations to the thermodynamic properties have been calculated using "air" as a single substance and adding the second and third virial corrections to existing or extrapolated values of these properties. Tables are given for the temperature range of 200 to 6000°K and for values of the common logarithm of the relative density up to 2.80, with (1) temperature and logarithm density and (2) temperature and entropy, as the independent variables.

(1962) Rosenbaum and Levitt (Ref. 27, 1962): This report presents hydrogen properties based upon a modified Altman truncation scheme which is an extension of Bethe's original proposal of truncating the partition function at a point where the classical electron orbit diameter approaches the distance between atoms. The above scheme takes into consideration the influence of the azimuthal quantum number upon the mean volume of the excited atom.

(1962) Hochstim and Terhune (Ref. 23, 1962): Properties of argon plasma to 100,000°K are presented. The computations were performed by an iterative technique so that the effect of Debye-Hückel corrections could be included to account for lowering of the ionization potential and termination of the partition function series.

(1962) Lick and Emmons (Ref. 17, 1962): Computations are presented of helium properties using the Unsöld theory to account for the partition function series truncation and ionization potential lowering. The results ran in pressures from 10^{-4} to 10^{3} atm for temperatures up to 50,000°K and are presented both in tabular and chart form. The authors compare the Unsöld, Bethe, and Debye truncation criterion. They conclude that the effect of ionization potential lowering and series truncation is less than a few percent, and that enthalpy, entropy, and composition would be accurate to within 10% if only ground states were considered. However, computations in which ionization potential lowering was examined indicated an error of about 30% in He^{+}concentrations at 30,000°K and a pressure of 100 atm. The error is reduced at higher and lower temperatures and is much smaller at lower pressures.

(1962) Raymond (Ref. 20, 1962): Calculation of equilibrium composition and Mollier data for CO_2 based upon ideal real-gas analysis for a pressure range of 10^{-4} to 10^{2} atm and temperature up to 24,000°K is presented.

(1962) Vale (Ref. 25, 1962) and Barnard and Hawkins (Ref. 24, 1962): These papers deal with computations of the composition of mixtures which involve multiphase products.

(1962) Michels and Schneidermen (Ref. 22, 1962): A method is presented for computing the high-temperature properties of mixtures in which the virial equation of state rather than the ideal equation of state is used to represent the components of the mixture. Comparisons of real and ideal behavior are presented for air, water gas and the H_2-O_2 system. The imperfect behavior is most pronounced at high pressure, i.e., about 100 to 1000 atm. Below this, the ideal or perfect real-gas assumption is valid.

(1962) Boynton (Ref. 21, 1962): An analysis is presented of the problem of calculating the equilibrium composition of an imperfect single-phase mixture. Computational techniques derived by the method of White, Johnson, and Dantzig and by the Newton-Raphson method are compared for gases obeying the virial equation of state. For the non-ideal or imperfect mixtures, the conclusion is that the Newton-Raphson method is simpler.

(1962) Rudin and Ragent (Ref. 26, 1962): A review of the state of the art, sources of discrepancy, and accuracy of thermodynamic computations for air is presented.

(1962) Marrone (Ref. 18, 1962): The (Ref. 36, 1959) work at NBS forms the basis for this tabulation of shock parameters in air.

(1961) Strahl (Ref. 32, 1961): A computation of thermodynamic properties and composition is presented for a model Venus atmosphere 85% CO_2–15% N_2 which is based upon perfect real-gas computations similar to the early air work of Gilmore at the Rand Corporation. The maximum temperature was 24,000°K.

(1961) Hochstim (Ref. 30, 1961): Ideal real-gas tabulations are presented of thermodynamic properties, chemical composition, and normal shock parameters for air with additional carbon, O_2, N_2, and CO_2. The thermochemistry is based upon early NBS tabulations. The maximum temperature was 10,000°K.

(1961) Stupochenko, Stakhanov, Samuilov, Pleshanov, and Rozhdestvenskii (Ref. 28, 1961): The authors present properties of air below 12,000°K over a sizable range of pressure. Particularly noteworthy in this work is the detailed analysis of the vibrational-rotational partition function and the estimates of those effects which were neglected. The authors used an ideal mixture assumption.

(1961) Sherman and Martinek (Ref. 29, 1961): This paper which is primarily concerned with the electrical transport properties of mercury presents some data on the thermodynamic property of this ionized gas. The method of Ecker and Weizel was used to account for the ionization potential lowering and electronic partition function truncation due to the micro field associated with the plasma. The authors present a comparison of the degree of ionization with a fixed arbitrary cut off and with the systematic treatment of the partition function, truncation, and ionization potential lowering. At 15,000°K the maximum difference of 3% occurs at the highest pressure considered, i.e., one atmosphere.

(1960) Wachman, Linevsky, and Lyon (Ref. 34, 1960): Computations were made using a perfect real-gas analysis to determine the properties of air-carbon mixtures. The equilibrium mixture contained 1 to 30% carbon by weight. Tabulations of equilibrium composition for a temperature range 4000° to 10,000°K and for pressure ranging from 0.1 to 100 atm are presented.

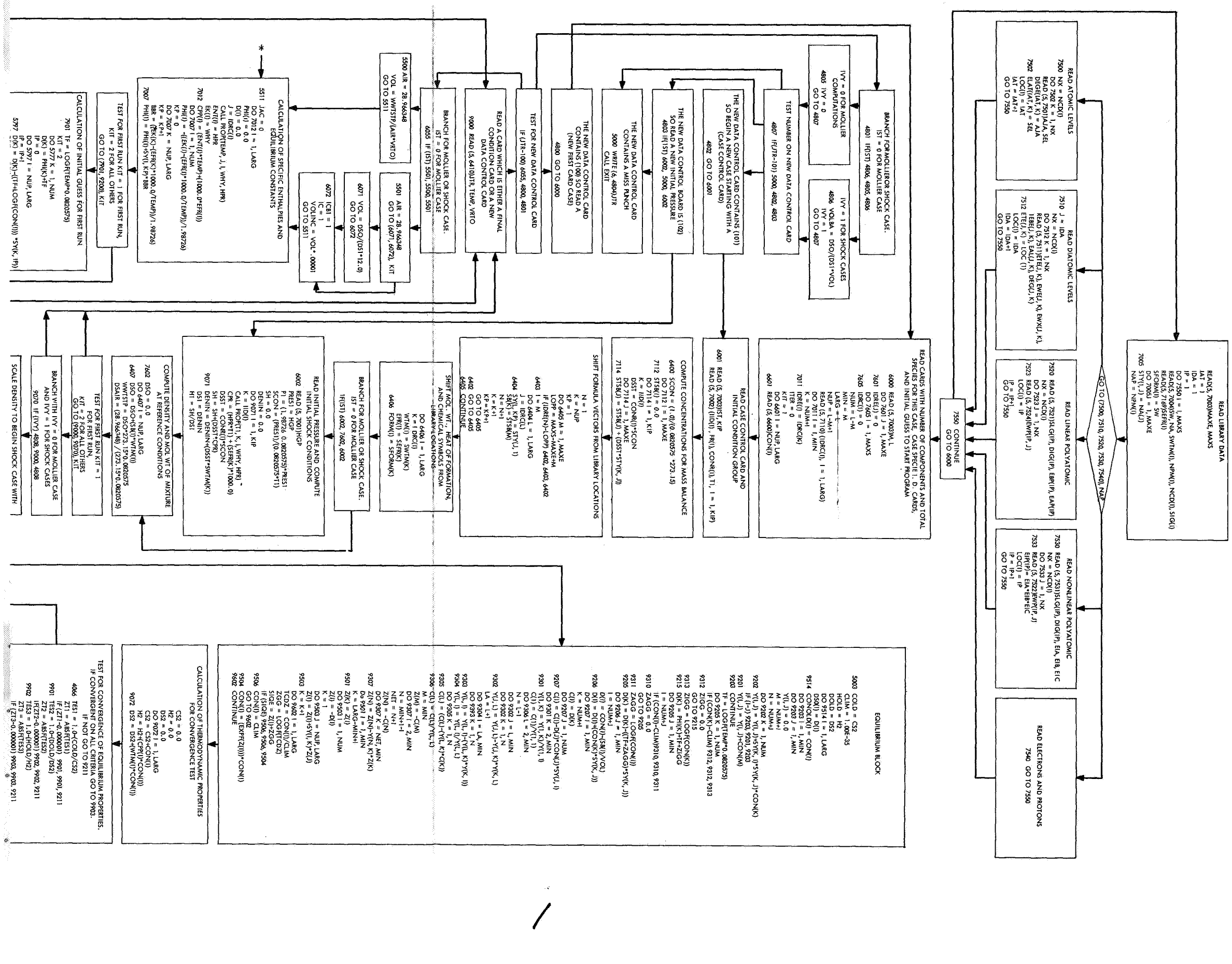
(1960) McGee and Heller (Ref. 16, 1960): Enthalpy and entropy tabulations as function of temperature and pressure are presented for hydrogen, helium, and lithium for temperatures up to 50,000°K. Their analysis takes into consideration imperfect gas behavior through the inclusion of the configuration integral term in the partition function. The potential used in its evaluation was based upon Debye-Hückel theory. Ionization potential lowering was based upon the work of Ecker and Weizel which is similar to the Unsöld theory. Truncation of the partition function sum is based upon the Inglis and Teller theory.

(1960) Brandmaier and Harnett (Ref. 35, 1960): A good survey of the techniques used for computing equilibrium composition of mixtures is presented.

(1959) Hilsenrath, Klein, and Woolley (Ref. 36, 1959): This earlier work at NBS treated air as an ideal or perfect real gas.

(1958) Rosher (Ref. 37, 1958): The author discussed the implicit and explicit assumptions made in computing the equilibrium composition of a gaseous mixture using the methods of statistical mechanics from available spectroscopic data.

Appendix B
Program Flow Diagram


READ LIBRARY DATA
GO TO (7500, 7510, 7520, 7530, 7540), NAP
READ ATOMIC LEVELS
READ DIATOMIC LEVELS
READ LINEAR POLYATOMIC
READ NONLINEAR POLYATOMIC
READ ELECTRONS AND PROTONS
7550 CONTINUE
GO TO 6000
READ CARDS WITH NUMBER OF COMPONENTS AN
SPECIES FOR THIS CASE, CASE SPECIFIC D. CA
AND INITIAL GUESS TO START PROGRAM
READ CASE CONTROL CARD AND
INITIAL CONDITION GROUP
COMPUTE CONCENTRATIONS FOR MASS BALA
SHIFT FORMULA VECTORS FROM LIBRARY LOCAT
EQUILIBRIUM BLOCK
BRANCH FOR MOLLIER OR SHOCK CASE:
IST = 0 FOR MOLLIER CASE
IVY = 0 FOR MOLLIER COMPUTATIONS
IVY = 1 FOR SHOCK CASES
TEST NUMBER ON NEW DATA CONTROL CARD
THE NEW DATA CONTROL CARD CONTAINS (101) SO BEGIN A NEW CASE STARTING WITH A (CASE CONTROL CARD)
THE NEW DATA CONTROL BOARD IS (102) SO READ A NEW INITIAL PRESSURE
THE NEW DATA CONTROL CARD CONTAINS A MISS PUNCH
THE NEW DATA CONTROL CARD CONTAINS (100) SO READ A NEW CASE (NEW FIRST CARD CASE)
TEST FOR NEW DATA CONTROL CARD
READ A CARD WHICH IS EITHER A FINAL CONDITION CARD OR A NEW DATA CONTROL CARD
BRANCH FOR MOLLIER OR SHOCK CASE:
IST = 0 FOR MOLLIER CASE
CALCULATION OF SPECIFIC ENTHALPIES AND EQUILIBRIUM CONSTANTS
TEST FOR FIRST RUN KIT = 1 FOR FIRST RUN, KIT = 2 FOR ALL OTHERS
GO TO (7901, 9200), KIT
CALCULATION OF INITIAL GUESS FOR FIRST RUN
READ INITIAL PRESSURE AND COMPUTE INITIAL SHOCK CONDITIONS
COMPUTE DENSITY AND MOL WT OF MIXTURE AT REFERENCE CONDITIONS
CALCULATION OF THERMODYNAMIC PROPERTIES FOR CONVERGENCE TEST
TEST FOR CONVERGENCE OF EQUILIBRIUM PROPERTIES. IF CONVERGENT ON ALL CRITERIA, GO TO 9903. IF NOT GO TO 9211
BRANCH WITH IVY = 0 FOR MOLLIER CASE AND IVY = 1 FOR SHOCK CASES
SCALE DENSITY TO BEGIN SHOCK CASE WITH

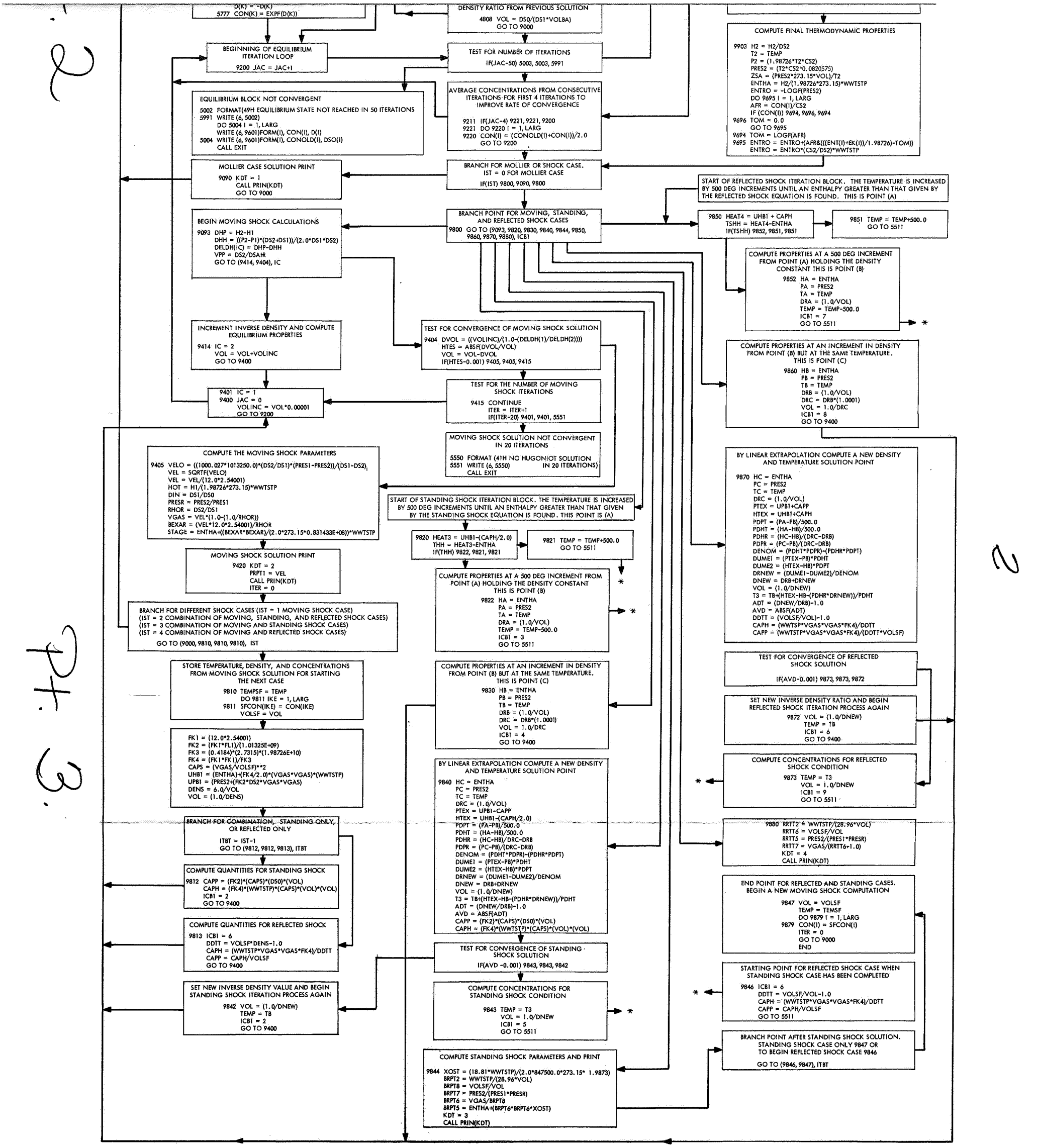


Fig. B-1. Program flow diagram

Appendix C

Key to Format Statements

I-format is used to enter fixed point numbers. The prefix numeral indicates the number of words. The suffix numeral indicates the number of spaces per word. For example, 2I3 is used to enter the numbers 5 and 416 in the following key punch form:

Word No. 1			Word No. 2		
0	0	5	4	1	6

F-format is used to enter floating point numbers for which the exponent notation is not needed to locate the decimal position. The prefix indicates the number of words. The suffix, which is a decimal, indicates the number of spaces per word and the number of digits from the right to the decimal position. For example, 3F5.3 is used to enter the numbers 0.72, 4.95 and 0.012 in the following key punch form:

Word No. 1					Word No. 2					Word No. 3				
0	.	7	2	0	4	.	9	5	0	0	.	0	1	2

E-format is used to enter floating point numbers for which the exponent notation is used to locate the decimal position. The prefix indicates the number of words. The suffix, which is a decimal number, indicates the number of spaces per word and the number of digits following the decimal. For example, 2E12.6 is used to enter the numbers 6.32×10^5 and .072 in the following key punch form:

Word No. 1																						
0	.	6	3	2	0	0	0	E	+	0	6	0	.	7	2	0	0	0	0	E	−	0	1

A-format is used to enter alpha-numeric data. The suffix is used to indicate the number of spaces per word. For example, A4 is used to enter CO_2 in the following key punch form:

	C	0	2

X-format is used for spacing. No values are read or printed.

Blanks in the key punch fields are read as zeros.

Appendix D
Program Listing and Description of Some of the Symbols and Fields Used in the Program

```
     0DIMENSION NA(10),SWTM(100),NPM(100),NCD(100),SEFR(100),SFORM(100),
     1STY(100,10),IDRC(100),IDRE(10),CON(100),IID(9),FR(9),CONR(9),
     2STSB(10),SY(100,10),Y(10,10),SB(100),WTM(100),EFR(100),FORM(100),
     3ENT(100),EK(100),CPP(100),PHI(100),D(100),C(100),Z(100),DSO(100),
     4CONOLD(100),DELDH(2),SFCON(100),SIG(100),ELAT(32,70),DEGE(32,70),
     5LOC(100),SLG(75),DIG(75),EBP(75),
     6EAP(75),EIP(75),EWP(75,12),ETE(20,10),EWE(20,10),
     7EWX(20,10),EBE(20,10),EAL(20,10),DEG(20,10)
      COMMON NPM, NCD,SIG,ELAT,DEGE,EWE,EWX,EBE,EAL,DEG,LOC,SLG,DIG,EBP
     1,EAP,EIP,EWP,ETE,SWTM,FORM,FR,CONR,CON,BRPT2,BRPT5,BRPT6,BRPT7,
     2BRPT8,CS2,DIN,DSAIR,DS2,ENTHA,ENTRO,HOT,PRESR,PRES1,PRES2,PRPT1,
     3RHOR,RRTT2,RRTT5,RRTT6,RRTT7,STAGE,TEMP,T1,VGAS,VRTO,WWTSTP,ZSA,
     4KIP,LARG
 4804 FORMAT(15H THE VALUE JTR=,I4,2X,12HIS NOT VALID)
 6410 FORMAT(1I3,2E12.6)
 6600 FORMAT(4X,1E12.6)
 7001 FORMAT(1E12.6)
 7002 FORMAT(I2,A6,1F7.5,1E12.6)
 7003 FORMAT(2I2)
 7004 FORMAT(12X,A6,10I2,1F10.6,I2,I4,1F4.1)
 7110 FORMAT(20I4)
 7169 FORMAT(20X,1E12.6)
 9601 FORMAT(3X,A4,2X,2E12.6)
 7501 FORMAT(17X,1F8.2,3X,1F10.3)
 7511 FORMAT(25X,1F11.4,1F9.3,1F10.5,1F10.6,1F9.6,1F6.2)
 7521 FORMAT(25X,2F3.1,2F8.5)
 7522 FORMAT(25X,1F8.2)
 7524 FORMAT(1F8.2)
 7531 FORMAT(25X,2F3.1,1F8.5,4X,1F8.5,4X,1F8.5,4X)
C
C         READ LIBRARY DATA
C
      READ INPUT TAPE 5,7003,MAXE,MAXS
      IAT=1
      IDA=1
      IP=1
      DO 7550 I=1,MAXS
      READ INPUT TAPE 5,7004,SW,NA,SWTM(I),NPM(I),NCD(I),SIG(I)
      READ INPUT TAPE 5,7169,SEFR(I)
      SFORM(I)=SW
      DO7005J=1,MAXE
 7005 STY(I,J)=NA(J)
      NAP=NPM(I)
      GO TO(7500,7510,7520,7530,7540),NAP
C
C         READ ATOMIC LEVELS
C
 7500 NX=NCD(I)
      DO 7502 K=1,NX
      READ INPUT TAPE 5,7501,AJA,SEL
      DEGE(IAT,K)=AJA
 7502 ELAT(IAT,K)=SEL
      LOC(I)=IAT
      IAT=IAT+1
      GO TO 7550
C
C         READ DIATOMIC LEVELS
C
```

```
 7510 J=IDA
      NX=NCD(I)
      DO 7512 K=1,NX
      READ INPUT TAPE 5,7511,ETE(J,K),EWE(J,K),EWX(J,K),
     1EBE(J,K),EAL(J,K),DEG(J,K)
 7512 ETE(J,K)=ETE(J,K)+(EWE(J,K)-EWE(J,1))*0.5-(EWX(J,K)-EWX(J,1))
     1*0.25
      LOC(I)=IDA
      IDA=IDA+1
      GO TO 7550
C
C       READ LINEAR POLYATOMIC
C
 7520 READ INPUT TAPE 5,7521,SLG(IP),DIG(IP),EBP(IP),EAP(IP)
      NX=NCD(I)
      DO 7523 J=1,NX
 7523 READ INPUT TAPE 5,7524,EWP(IP,J)
      LOC(I)=IP
      IP=IP+1
      GO TO 7550
C
C         READ NONLINEAR POLYATOMIC
C
 7530 READ INPUT TAPE 5,7531,SLG(IP),DIG(IP),EIA,EIB,EIC
      NX=NCD(I)
      DO 7533 J=1,NX
 7533 READ INPUT TAPE 5,7522,EWP(IP,J)
      EIP(IP)=EIA*EIB*EIC
      LOC(I)=IP
      IP=IP+1
      GO TO 7550
C
C         READ ELECTRONS AND PROTONS
C
 7540 GO TO 7550
 7550 CONTINUE
      GO TO 6000
C
C          READ CARDS WITH NUMBER OF COMPONENTS AND TOTAL SPECIES FOR THIS
C          CASE ,CASE SPECIE I. D. CARDS, AND INITIAL GUESS TO START PROGRAM
C
 6000 READ INPUT TAPE 5,7003,M,L
      DO 7601 J=1,MAXE
 7601 IDRE(J)=0
      DO 7605 I=1,MAXS
 7605 IDRC(I)=0
      NUM=L-M
      MIN=M
      LARG=L
      NUP=L-M+1
      READ INPUT TAPE 5,7110,(IDRC(I),I=1,LARG)
      DO 7011 I=1,MIN
      K=NUM+I
 7011 IDRE(I)=IDRC(K)
      ITER=0
      KIT=1
      DO 6601 I=NUP,LARG
 6601 READ INPUT TAPE 5,6600,CON(I)
C
```

```
C          READ CASE CONTROL CARD AND INITIAL CONDITION GROUP
C
 6001 READ INPUT TAPE 5,7003,IST,KIP
      READ INPUT TAPE 5,7002,(IID(I),FR(I),CONR(I),T1,I=1,KIP)
C
C          COMPUTE CONCENTRATIONS FOR MASS BALANCE
C
 6400 SCON=(1.0)/(0.0820575*273.15)
      DO 7112 I=1,MAXE
 7112 STSB(I)=0.0
      DO 7114 I=1,KIP
      K=IID(I)
      DSST=CONR(I)*SCON
      DO 7114 J=1,MAXE
 7114 STSB(J)=STSB(J)+(DSST*STY(K,J))
C
C          SHIFT FORMULA VECTORS FROM LIBRARY LOCATIONS
C
      N=1
      K=NUP
      KP=1
      DO 6405 M=1,MAXE
      LOPP=MAXS-MAXE+M
      IF (IDRE(N)-LOPP) 6402,6403,6402
 6403 I=M
      DO 6404 L=1,LARG
      J=IDRC(L)
 6404 SY(L,KP)=STY(J,I)
      SB(K)=STSB(M)
      N=N+1
      K=K+1
      KP=KP+1
      GO TO 6405
 6402 GO TO 6405
 6405 CONTINUE
C
C          SHIFT MOL. WT., HEAT OF FORMATION , AND CHEMICAL SYMBOLS FROM
C          LIBRARY LOCATIONS
C
      DO 6406 I=1,LARG
      K=IDRC(I)
      WTM(I)=SWTM(K)
      EFR(I)=SEFR(K)
 6406 FORM(I)=SFORM(K)
C
C          BRANCH FOR MOLLIER OR SHOCK CASE. IST=0 FOR MOLLIER CASE
C
      IF(IST) 6002,7602,6002
C
C          READ INITIAL PRESSURE AND COMPUTE INITIAL SHOCK CONDITIONS
C
 6002 READ INPUT TAPE 5,7001,HGP
      PRES1=HGP
      P1=(1.98726/0.0820575)*PRES1
      SCON=(PRES1)/(0.0820575*T1)
      SH=0.0
      DENIN=0.0
      DO 9071 I=1,KIP
      K=IID(I)
```

```
      CALL PROP(T1,K,I,WHY,HPR)
      CPR=(HPR*T1)+(SEFR(K)*1000.0)
      DSST=CONR(I)*SCON
      SH=SH+(DSST*CPR)
 9071 DENIN=DENIN+(DSST*SWTM(K))
      DS1=DENIN
      H1=SH/DS1
C
C         COMPUTE DENSITY AND MOL WT OF MIXTURE AT REFERENCE CONDITIONS
C
 7602 DS0=0.0
      DO6407 I=NUP,LARG
 6407 DS0=DS0+(SB(I)*WTM(I))
      WWTSTP=DS0*273.15*0.0820575
      DSAIR=(28.966348)/(273.15*0.0820575)
C
C        TEST FOR FIRST RUN KIT=1 FOR FIRST RUN,KIT=2 FOR ALL OTHERS
C
      GO TO(9000,9070),KIT
C
C         BRANCH WITH IVY=0 FOR MOLLIER CASE AND IVY=1 FOR SHOCK CASES
C
 9070 IF(IVY) 4808,9000,4808
C
C         SCALE DENSITY TO BEGIN SHOCK CASE WITH DENSITY RATIO FROM PREVIOUS
C         SOLUTION
C
 4808 VOL=DS0/(DS1*VOLBA)
      GO TO 9000
C
C         READ A CARD WHICH IS EITHER A FINAL CONDITION CARD OR A NEW DATA
C         CONTROL CARD
C
 9000 READ INPUT TAPE 5, 6410,JTR,TEMP,VRTO
C
C         TEST FOR NEW DATA CONTROL CARD
C
      IF(JTR-100)6055,4800,4801
C
C         THE NEW DATA CONTROL CARD CONTAINS (100)SO READ A(NEW FIRST CARD CASE)
C
 4800 GO TO 6000
C
C         BRANCH FOR MOLLIER OR SHOCK CASE. IST=0 FOR MOLLIER CASE
C
 4801 IF(IST) 4806,4805,4806
C
C         IVY=0 FOR MOLLIER COMPUTATIONS
C
 4805 IVY=0
      GO TO 4807
C
C         IVY=1 FOR SHOCK CASES
C
 4806 VOLBA=DS0/(DS1*VOL)
      IVY=1
      GO TO 4807
C
C         TEST NUMBER ON NEW DATA CONTROL CARD
```

```
C
 4807 IF(JTR-101) 5000,4802,4803
C
C          THE NEW DATA CONTROL CARD CONTAINS(101) SO BEGIN A NEW CASE STARTING
C          WITH A (CASE CONTROL CARD)
C
 4802 GO TO 6001
C
C          THE NEW DATA CONTROL CARD IS (102) SO READ A NEW INITIAL PRESSURE
C
 4803 IF (IST) 6002,5000,6002
C
C          THE NEW DATA CONTROL CARD CONTAINS A MISS PUNCH
C
 5000 WRITE OUTPUT TAPE 6,4804,JTR
      CALL EXIT
C
C          BRANCH FOR MOLLIER OR SHOCK CASE. IST=0 FOR MOLLIER CASE
C
 6055 IF(IST)5501,5500,5501
 5500 AIR=28.966348
      VOL=WWTSTP/(AIR*VRTO)
      GO TO 5511
 5501 AIR=28.966348
      GO TO(6071,6072),KIT
 6071 VOL=DS0/(DS1*12.0)
      GO TO 6072
 6072 ICB1=1
      IC=1
      VOLINC=VOL*.00001
      GO TO 5511
C
C        CALCULATION OF SPECIFIC ENTHALPIES AND EQUILIBRIUM CONSTANTS
C
 5511 JAC=0
      DO 7012 I=1,LARG
      PHI(I)=0.0
      D(I)=0.0
      J=IDRC(I)
      CALL PROP(TEMP,J,I,WHY,HPR)
      ENT(I)=HPR
      EK(I)=WHY
 7012 CPP(I)=(ENT(I)*TEMP)+(1000.0*EFR(I))
      DO 7007 I=1,NUM
      PHI(I)= -((EK(I)-(EFR(I)*1000.0/TEMP))/1.98726)
      KP=0
      DO 7007 K=NUP,LARG
      KP=KP+1
      BBR=((EK(K)-(EFR(K)*1000.0/TEMP))/1.98726)
 7007 PHI(I)=PHI(I) +SY(I,KP)*BBR
C
C        TEST FOR FIRST RUN KIT=1 FOR FIRST RUN,KIT=2 FOR ALL OTHERS
C
      GO TO(7901,9200),KIT
C
C        CALCULATION OF INITIAL GUESS FOR FIRST RUN
C
 7901 TF=LOGF(TEMP*0.0820575)
      KIT=2
```

```
      DO 5777 K=1,NUM
      D(K)=PHI(K)+TF
      IP=0
      DO 5797 I=NUP,LARG
      IP=IP+1
 5797 D(K)=D(K)-((TF+LOGF(CON(I)))*SY(K,IP))
      D(K)=-D(K)
 5777 CON(K)=EXPF(D(K))
C
C        BEGINNING OF EQUILIBRIUM ITERATION LOOP
C
 9200 JAC=JAC+1
C
C        TEST FOR NUMBER OF ITERATIONS
C
      IF(JAC-50) 5003, 5003, 5991
C
C        EQUILIBRIUM BLOCK NOT CONVERGENT
C
 5002 FORMAT(49H EQUILIBRIUM STATE NOT REACHED IN 50 ITERATIONS)
 5991 WRITE OUTPUT TAPE 6,5002
      DO 5004 I=1,LARG
      WRITE OUTPUT TAPE 6,9601,FORM(I),CON(I),D(I)
 5004 WRITE OUTPUT TAPE 6,9601,FORM(I),CONOLD(I),DSO(I)
      CALL EXIT
C
C        EQUILIBRIUM BLOCK
C
 5003 COLD=CS2
      CLIM=1.00E-35
      HOLD=H2
      DOLD=DS2
      DO 9514 I=1,LARG
      DSO(I)=D(I)
 9514 CONOLD(I)=CON(I)
      DO 9203 I=1,MIN
      DO 9203 J=1,MIN
      Y(I,J)=0.0
      M=NUM+I
      N=NUM+J
      DO 9202 K=1,NUM
 9202 Y(I,J)=Y(I,J)+SY(K,I)*SY(K,J)*CON(K)
      IF(I-J) 9203,9201,9203
 9201 Y(I,J)=Y(I,J)+CON(M)
 9203 CONTINUE
      TF=LOGF(TEMP*0.0820575)
      DO 9205 K=1,NUM
      IF(CON(K)-CLIM)9312,9312,9313
 9312 ZIGG=LOGF(CLIM)
      GO TO 9215
 9313 ZIGG=LOGF(CON(K))
 9215 D(K)=PHI(K)+TF+ZIGG
      DO 9205 J=1,MIN
      I=NUM+J
      IF(CON(I)-CLIM)9310,9310,9311
 9310 ZAGG=LOGF(CLIM)
      GO TO 9205
 9311 ZAGG=LOGF(CON(I))
 9205 D(K)=D(K)-((TF+ZAGG)*SY(K,J))
```

```
      DO 9206 J=1,MIN
      I=NUM+J
      D(I)=CON(I)-(SB(I)/VOL)
      DO 9206 K=1,NUM
 9206 D(I)=D(I)+(CON(K)*SY(K,J))
      DO 9207 I=1,MIN
      K=NUM+I
      C(I)=D(K)
      DO 9207 J=1,NUM
 9207 C(I)=C(I)-D(J)*CON(J)*SY(J,I)
      DO 9301 K=2,MIN
 9301 Y(1,K)=Y(1,K)/Y(1,1)
      C(1)=C(1)/Y(1,1)
      DO 9306 L=2,MIN
      N=L-1
      DO 9302 J=L,MIN
      DO 9302 K=1,N
 9302 Y(J,L)=Y(J,L)-Y(J,K)*Y(K,L)
      LA=L+1
      DO 9304 I=LA,MIN
      DO 9303 K=1,N
 9303 Y(L,I)=Y(L,I)-(Y(L,K)*Y(K,I))
 9304 Y(L,I)=Y(L,I)/Y(L,L)
      DO 9305 K=1,N
 9305 C(L)=C(L)-(Y(L,K)*C(K))
 9306 C(L)=C(L)/Y(L,L)
      M=MIN
      Z(M)=-C(M)
      DO 9307 I=2,MIN
      N=MIN+1-I
      NET=N+1
      Z(N)=-C(N)
      DO 9307 K=NET,MIN
 9307 Z(N)=Z(N)-Y(N,K)*Z(K)
      DO 9501 I=1,MIN
      K=LARG-MIN+I
 9501 Z(K)=Z(I)
      DO 9503 I=1,NUM
      Z(I)=-D(I)
      K=1
      DO 9503 J=NUP,LARG
      Z(I)=Z(I)+SY(I,K)*Z(J)
 9503 K=K+1
      DO 9602 I=1,LARG
      TCDZ=CON(I)/CLIM
      ZGG=LOGF(TCDZ)
      SIQE=Z(I)+ZGG
      IF(SIQE) 9506,9506,9504
 9506 CON(I)=CLIM
      GO TO 9602
 9504 CON(I)=(EXPF(Z(I)))*CON(I)
 9602 CONTINUE
C
C          CALCULATION OF THERMODYNAMIC PROPERTIES FOR CONVERGENCE TEST
C
      CS2=0.0
      H2=0.0
      DS2=0.0
      DO 9072 I=1,LARG
```

```
      CS2=CS2+CON(I)
      H2=H2+(CPP(I)*CON(I))
 9072 DS2=DS2+(WTM(I)*CON(I))
C
C         TEST FOR CONVERGENCE OF EQUILIBRIUM PROPERTIES.  IF CONVERGENT ON ALL
C         CRITERIA GO TO 9903. IF NOT GO TO 9211
C
 4066 TES1=1.0-(COLD/CS2)
      ZT1=ABSF(TES1)
      IF(ZT1-0.000001) 9901, 9901, 9211
 9901 TES2=1.0-(DOLD/DS2)
      ZT2=ABSF(TES2)
      IF(ZT2-0.000001) 9902, 9902, 9211
 9902 TES3=1.0-(HOLD/H2)
      ZT3=ABSF(TES3)
      IF(ZT3-0.000001) 9903, 9903, 9211
C
C         AVERAGE CONCENTRATIONS FROM CONSECUTIVE ITERATIONS FOR FIRST 4
C         ITERATIONS TO IMPROVE RATE OF CONVERGENCE
C
 9211 IF(JAC-4) 9221,9221,9200
 9221 DO 9220 I=1,LARG
 9220 CON(I)=(CONOLD(I)+CON(I))/2.0
      GO TO 9200
C
C         COMPUTE FINAL THERMODYNAMIC PROPERTIES
C
 9903 H2=H2/DS2
      T2=TEMP
      P2=(1.98726*T2*CS2)
      PRES2=(T2*CS2*0.0820575)
      ZSA=(PRES2*273.15*VOL)/T2
      ENTHA=H2/(1.98726*273.15)*WWTSTP
      ENTRO=-LOGF(PRES2)
      DO 9695 I=1,LARG
      AFR=CON(I)/CS2
      IF(CON(I))9694,9696,9694
 9696 TOM=0.0
      GO TO 9695
 9694 TOM=LOGF(AFR)
 9695 ENTRO=ENTRO+(AFR*(((ENT(I) +EK(I))/1.98726)-TOM))
      ENTRO=ENTRO*(CS2/DS2)*WWTSTP
C
C         BRANCH FOR MOLLIER OR SHOCK CASE. IST=0 FOR MOLLIER CASE
C
      IF(IST) 9800,9090,9800
C
C         BRANCH POINT FOR MOVING, STANDING, AND REFLECTED SHOCK CASES
C
 9800 GO TO (9093,9820,9830,9840,9844,9850,9860,9870,9880),ICB1
C
C         BEGIN MOVING SHOCK CALCULATIONS
C
 9093 DHP=H2-H1
      DHH=((P2-P1)*(DS2+DS1))/(2.0*DS1*DS2)
      DELDH(IC)=DHP-DHH
      VPP=DS2/DSAIR
      GO TO ( 9414, 9404),IC
C
```

```
C          INCREMENT INVERSE DENSITY AND COMPUTE EQUILIBRIUM PROPERTIES
C
 9414 IC=2
      VOL=VOL+VOLINC
      GO TO 9400
 9401 IC=1
 9400 JAC=0
      VOLINC=VOL*.00001
      GO TO 9200
C
C          TEST FOR CONVERGENCE OF MOVING SHOCK SOLUTION
C
 9404 DVOL=((VOLINC)/(1.0-(DELDH(1)/DELDH(2))))
      HTES=ABSF(DVOL/VOL)
      VOL=VOL-DVOL
      IF(HTES-0.001  )9405,9405,9415
C
C          TEST FOR THE NUMBER OF MOVING SHOCK ITERATIONS
C
 9415 CONTINUE
      ITER=ITER+1
      IF(ITER-20)9401,9401,5551
C
C          MOVING SHOCK SOLUTION NOT CONVERGENT IN 20 ITERATIONS
C
 5550 FORMAT (41H   NO HUGONIOT SOLUTION IN 20 ITERATIONS )
 5551 WRITE OUTPUT TAPE 6, 5550
      CALL EXIT
C
C          COMPUTE THE MOVING SHOCK PARAMETERS
C
 9405 VELO=((1000.027*1013250.0)*(DS2/DS1)*(PRES1-PRES2))/(DS1-DS2)
      VEL=SQRTF(VELO)
      VEL=VEL/(12.0*2.54001)
      HOT=H1/(1.98726*273.15)*WWTSTP
      DIN=DS1/DS0
      PRESR=PRES2/PRES1
      RHOR=DS2/DS1
      VGAS=VEL*(1.0-(1.0/RHOR))
      BEXAR=(VEL*12.0*2.54001)/RHOR
      STAGE=ENTHA+((BEXAR*BEXAR)/(2.0*273.15*0.831433E+08))*WWTSTP
C
C          MOVING SHOCK SOLUTION PRINT
C
 9420 KDT=2
      PRPT1=VEL
      CALL PRIN(KDT)
      ITER=0
C
C          BRANCH FOR DIFFERENT SHOCK CASES (IST=1 MOVING SHOCK CASE)
C          (IST=2 COMBINATION OF MOVING ,STANDING ,AND REFLECTED SHOCK CASES)
C          (IST=3 COMBINATION OF MOVING AND STANDING SHOCK CASES)
C          (IST=4 COMBINATION OF MOVING AND REFLECTED SHOCK CASES)
C
      GO TO(9000,9810,9810,9810),IST
C
C          MOLLIER CASE SOLUTION PRINT
C
 9090 KDT=1
```

```
      CALL PRIN(KDT)
      GO TO 9000
C
C          STORE QUANTITIES FROM MOVING SHOCK SOLUTION FOR NEXT CASE
C
 9810 TEMPSF=TEMP
      DO 9811 IKE=1,LARG
 9811 SFCON(IKE)=CON(IKE)
      VOLSF=VOL
      FK1=(12.0*2.54001)
      FK2=(FK1*FK1)/(1.01325E+09)
      FK3=(0.4184)*(2.7315)*(1.98726E+10)
      FK4=(FK1*FK1)/FK3
      CAPS=(VGAS/VOLSF)**2
      UHB1=(ENTHA)+(FK4/2.0)*(VGAS*VGAS)*(WWTSTP)
      UPB1= PRES2 +(FK2*DS2*VGAS*VGAS)
      DENS=6.0/VOL
      VOL=(1.0/DENS)
C
C          BRANCH FOR COMBINATION SHOCK, STANDING SHOCK, OR REFLECTED SHOCK
C
      ITBT=IST-1
      GO TO(9812,9812,9813),ITBT
C
C          COMPUTE QUANTITIES FOR STANDING SHOCK
C
 9812 CAPP=(FK2)*(CAPS)*(DS0)*(VOL)
      CAPH=(FK4)*(WWTSTP)*(CAPS)*(VOL)*(VOL)
      ICB1=2
      GO TO 9400
C
C          COMPUTE QUANTITIES FOR REFLECTED SHOCK
C
 9813 ICB1=6
      DDTT=VOLSF*DENS-1.0
      CAPH=(WWTSTP*VGAS*VGAS*FK4)/DDTT
      CAPP=CAPH/VOLSF
      GO TO 9400
C
C          START OF STANDING  SHOCK ITERATION BLOCK. THE TEMPERATURE IS INCREASED
C          BY 500 DEG INCREMENTS UNTIL AN ENTHALPY GREATER THAN THAT GIVEN BY THE
C          STANDING  SHOCK EQUATION IS FOUND. THIS IS POINT(A)
C
 9820 HEAT3= UHB1-(CAPH/2.0)
      THH=HEAT3-ENTHA
      IF(THH) 9822,9821,9821
 9821 TEMP=TEMP+500.0
      GO TO 5511
C
C          COMPUTE PROPERTIES AT A 500 DEG INCREMENT FROM POINT (A) HOLDING
C          THE DENSITY CONSTANT THIS IS POINT (B)
C
 9822 HA=ENTHA
      PA=PRES2
      TA=TEMP
      DRA=(1.0/VOL)
      TEMP=TEMP-500.0
      ICB1=3
      GO TO 5511
```

```
C
C          COMPUTE PROPERTIES AT AN INCREMENT IN DENSITY FROM POINT (B) BUT
C          AT THE SAME TEMPERATURE. THIS IS POINT (C)
C
 9830 HB=ENTHA
      PB=PRES2
      TB=TEMP
      DRB=(1.0/VOL)
      DRC=DRB*(1.0001)
      VOL=1.0/DRC
      ICB1=4
      GO TO 9400
C
C          BY LINEAR EXTRAPOLATION COMPUTE A NEW DENSITY AND TEMPERATURE
C          SOLUTION POINT
C
 9840 HC=ENTHA
      PC=PRES2
      TC=TEMP
      DRC=(1.0/VOL)
      PTEX=UPB1-CAPP
      HTEX=UHB1-(CAPH/2.0)
      PDPT=(PA-PB)/500.0
      PDHT=(HA-HB)/500.0
      PDHR=(HC-HB)/(DRC-DRB)
      PDPR=(PC-PB)/(DRC-DRB)
      DENOM=(PDHT*PDPR)-(PDHR*PDPT)
      DUME1=(PTEX-PB)*PDHT
      DUME2=(HTEX-HB)*PDPT
      DRNEW=(DUME1-DUME2)/DENOM
      DNEW=DRB+DRNEW
      VOL=(1.0/DNEW)
      T3=TB+(HTEX-HB-(PDHR*DRNEW))/PDHT
      ADT=(DNEW/DRB)-1.0
      AVD=ABSF(ADT)
      CAPP=(FK2)*(CAPS)*(DS0)*(VOL)
      CAPH=(FK4)*(WWTSTP)*(CAPS)*(VOL)*(VOL)
C
C          TEST FOR CONVERGENCE OF STANDING SHOCK SOLUTION
C
      IF(AVD-0.001) 9843,9843,9842
C
C          SET NEW INVERSE DENSITY  VALUE AND BEGIN STANDING SHOCK
C          ITERATION PROCESS AGAIN
C
 9842 VOL=(1.0/DNEW)
      TEMP=TB
      ICB1=2
      GO TO 9400
C
C          COMPUTE CONCENTRATIONS FOR STANDING SHOCK CONDITION
C
 9843 TEMP=T3
      VOL=1.0/DNEW
      ICB1=5
      GO TO 5511
C
C          COMPUTE STANDING SHOCK PARAMETERS AND PRINT
C
```

```
 9844 XOST=(18.81*WWTSTP)/(2.0*847500.0*273.15*1.9873)
      BRPT2=WWTSTP/(28.96*VOL)
      BRPT8=VOLSF/VOL
      BRPT7=PRES2/(PRES1*PRESR)
      BRPT6=VGAS/BRPT8
      BRPT5=ENTHA+(BRPT6*BRPT6*XOST)
      KDT=3
      CALL PRIN(KDT)
C
C         BRANCH POINT AFTER STANDING SHOCK SOLUTION. STANDING SHOCK CASE
C         ONLY 9847 OR TO BEGIN REFLECTED SHOCK CASE 9846
C
      GO TO (9846,9847),ITBT
C
C         STARTING POINT FOR REFLECTED SHOCK CASE WHEN STANDING SHOCK CASE HAS
C         BEEN COMPLETED
C
 9846 ICB1=6
      DDTT=VOLSF/VOL-1.0
      CAPH=(WWTSTP*VGAS*VGAS*FK4)/DDTT
      CAPP=CAPH/VOLSF
      GO TO 5511
C
C         START OF REFLECTED SHOCK ITERATION BLOCK. THE TEMPERATURE IS INCREASED
C         BY 500 DEG INCREMENTS UNTIL AN ENTHALPY GREATER THAN THAT GIVEN BY THE
C         REFLECTED SHOCK EQUATION IS FOUND. THIS IS POINT(A)
C
 9850 HEAT4=UHB1+CAPH
      TSHH=HEAT4-ENTHA
      IF(TSHH) 9852,9851,9851
 9851 TEMP=TEMP+500.0
      GO TO 5511
C
C         COMPUTE PROPERTIES AT A 500 DEG INCREMENT FROM POINT (A) HOLDING
C         THE DENSITY CONSTANT THIS IS POINT (B)
C
 9852 HA=ENTHA
      PA=PRES2
      TA=TEMP
      DRA=(1.0/VOL)
      TEMP=TEMP-500.0
      ICB1=7
      GO TO 5511
C
C         COMPUTE PROPERTIES AT AN INCREMENT IN DENSITY FROM POINT (B) BUT
C         AT THE SAME TEMPERATURE. THIS IS POINT (C)
C
 9860 HB=ENTHA
      PB=PRES2
      TB=TEMP
      DRB=(1.0/VOL)
      DRC=DRB*(1.0001)
      VOL=1.0/DRC
      ICB1=8
      GO TO 9400
C
C         BY LINEAR EXTRAPOLATION COMPUTE A NEW DENSITY AND TEMPERATURE
C         SOLUTION POINT
C
```

```
 9870 HC=ENTHA
      PC=PRES2
      TC=TEMP
      DRC=(1.0/VOL)
      PTEX=UPB1+CAPP
      HTEX=UHB1+CAPH
      PDPT=(PA-PB)/500.0
      PDHT=(HA-HB)/500.0
      PDHR=(HC-HB)/(DRC-DRB)
      PDPR=(PC-PB)/(DRC-DRB)
      DENOM=(PDHT*PDPR)-(PDHR*PDPT)
      DUME1=(PTEX-PB)*PDHT
      DUME2=(HTEX-HB)*PDPT
      DRNEW=(DUME1-DUME2)/DENOM
      DNEW=DRB+DRNEW
      VOL=(1.0/DNEW)
      T3=TB+(HTEX-HB-(PDHR*DRNEW))/PDHT
      ADT=(DNEW/DRB)-1.0
      AVD=ABSF(ADT)
      DDTT=(VOLSF/VOL)-1.0
      CAPH=(WWTSTP*VGAS*VGAS*FK4)/DDTT
      CAPP=(WWTSTP*VGAS*VGAS*FK4)/(DDTT*VOLSF)
C
C         TEST FOR CONVERGENCE OF REFLECTED SHOCK SOLUTION
C
      IF(AVD-0.001) 9873,9873,9872
C
C         SET NEW INVERSE DENSITY  RATIO AND BEGIN  REFLECTED SHOCK
C         ITERATION PROCESS AGAIN
C
 9872 VOL=(1.0/DNEW)
      TEMP=TB
      ICB1=6
      GO TO 9400
C
C         COMPUTE CONCENTRATIONS FOR REFLECTED SHOCK CONDITION
C
 9873 TEMP=T3
      VOL=1.0/DNEW
      ICB1=9
      GO TO 5511
C
C         COMPUTE REFLECTED SHOCK PARAMETERS AND PRINT
C
 9880 RRTT2=WWTSTP/(28.96*VOL)
      RRTT6=VOLSF/VOL
      RRTT5=PRES2/(PRES1*PRESR)
      RRTT7=VGAS/(RRTT6-1.0)
      KDT=4
      CALL PRIN(KDT)
C
C         END POINT FOR REFLECTED AND STANDING CASES. BEGIN A NEW MOVING
C         SHOCK COMPUTATION
C
 9847 VOL=VOLSF
      TEMP=TEMSF
      DO 9879 I=1,LARG
 9879 CON(I)=SFCON(I)
      ITER=0
```

```
      GO TO 9000
      END
C        SUBROUTINE FOR THERMOCHEMICAL PROPERTIES
      SUBROUTINE PROP(TDC,I,K,PEK,PENT)
      DIMENSION NPM(100),NCD(100),EAP(75),EIP(75),EWP(75,12),ETE(20,10),
     1EWE(20,10),EWX(20,10),EBE(20,10),EAL(20,10),DEG(20,10),SIG(100),
     2DEGE(32,70),LOC(100),SLG(75),DIG(75),EBP(75),ELAT(32,70),SWTM(100)
      COMMON NPM, NCD,SIG,ELAT,DEGE,EWE,EWX,EBE,EAL,DEG,LOC,SLG,DIG,EBP
     1,EAP,EIP,EWP,ETE,SWTM
C       TDC=TEMPERATURE
C       I=I.D.NUMBER FOR SPECIE IN INPUT LIST
C       K=I.D.NUMBER FOR THE ORDER OF THE SPECIE  IN EQUILIBRIUM COMPUTATION
C      PENT=(H-HO)/T
C      PEK=-(F-HO)/T
C       DEG(I,J)=DEGENERACY OF THE J,TH ENERGY LEVEL FOR I,TH SPECIE
C       EL(I,J)=J,TH ENERGY LEVEL FOR I,TH SPECIE
      THA=(1.3804*TDC)/(2.99793*0.66252)
      PGR=1.98726
      IBB=NPM(I)
      GO TO(5711,5721,5731,5741,5751),IBB
C        COMPUTATIONFOR ATOMIC THERMOCHEMICAL PROPERTIES
 5711 BLB=20.0
      ELL=2.3026*BLB*THA
      J=1
      L=LOC(I)
      PAR=0.0
      HNT=0.0
 5700 IF(ELAT(L,J)-ELL) 5710,5710,5720
 5710 VTV=DEGE(L,J)*EXPF(-ELAT(L,J)/THA)
      PAR=PAR+VTV
      HNT=HNT+(ELAT(L,J)*VTV)
      J=J+1
      IF(J-NCD(I))5700,5700,5720
 5720 PENT  =PGR*(2.5+((HNT)/(PAR*THA)))
      AB=LOGF(PAR)
      BB=LOGF(SWTM(I))
      CB=LOGF(TDC)
      PEK  =PGR*((2.5*CB)+(1.5*BB)+AB)-7.28353
      GO TO 5790
C       COMPUTATION FOR DIATOMIC PROPERTIES
 5721 A=SWTM(I)
      L=LOC(I)
      W=EWE(L,1)-(2.0*EWX(L,1))
      BBB=EBE(L,1)-(0.5*EAL(L,1))
      B=(2.99793*0.66252*BBB)/(1.3804)
      G= DEG(L,1)/SIG(I)
      AA=LOGF(A)
      CC=LOGF(G)
      BB=LOGF(B)
      E=1.5*AA-BB+CC
      ENF=(PGR*E)-7.28353
      T=LOGF(TDC)
      TR=3.5*PGR*T
      ENF=ENF+TR
      U=W/THA
      EU=EXPF(U)
      EUD=EU-1.0
      TED=EU/EUD
      TL=LOGF(TED)
```

```
      PEK=ENF+(PGR*TL)
      PENT=PGR*(3.5+(U/EUD))
      CEK=1.0
      CEN=0.0
      NX=NCD(I)
      DO 5722 IH=2,NX
      G=EXPF(-ETE(L,IH)/THA)
      TL=(DEG(L,IH)*G)/DEG(L,1)
      CEK=CEK+TL
 5722 CEN=CEN+(TL*ETE(L,IH))
      AA=LOGF(CEK)
      BB=CEN/CEK
      PEK=PEK+(AA*PGR)
      PENT=PENT+((BB*PGR)/THA)
      A=EBE(L,1)/EWE(L,1)
      B=EAL(L,1)/EBE(L,1)
      AA=EWX(L,1)/EWE(L,1)
      BB=(8.0*A)/U
      BF2=B/EUD
      BF3=(2.0*AA*U)/(EUD*EUD)
      BE2=((U*B*EU)-(2.0*U*AA))/(EUD*EUD)
      BE3=(4.0*AA*U*U*EU)/(EUD*EUD*EUD)
      CEK=PGR*(BB+BF2+BF3)
      CEN=PGR*(BB+BE2+BE3)
      PEK=PEK+CEK
      PENT=PENT+CEN
      GO TO 5790
C        COMPUTATION FOR  LINEAR POLYATOMIC PROPERTIES
 5731 EN=3.5*PGR
      ENF=-7.28353
      A=SWTM(I)
      L=LOC(I)
      G=DIG(L)/SLG(L)
      BB=LOGF(G)
      AB=LOGF(A)
      AA=PGR*((1.5*AB)+BB)
      ENF=ENF+AA
      BBB=EBP(L)-(0.5*EAP(L))
      B=(2.99793*0.66252*BBB)/(1.3804)
      BB=LOGF(B)
      AA=PGR*BB
      ENF=ENF-AA
      ET=LOGF(TDC)
      AB=ET*PGR*3.5
      ENF=ENF+AB
      N=NCD(I)
      DO 7532 J=1,N
      U=EWP(L,J)/THA
      EU=EXPF(U)
      EUD=EU-1.0
      EP=EU/EUD
      EH=U/EUD
      EL=LOGF(EP)
      EHR=PGR*EH
      ELR=PGR*EL
      EN=EN+EHR
 7532 ENF=ENF+ELR
      PEK=ENF
      PENT=EN
```

```
      GO TO 5790
C       COMPUTATION FOR NONLINEAR POLYATOMIC PROPERTIES
 5741 EN=4.0
      ENF=0.0
      A=SWTM(I)
      L=LOC(I)
      B=EIP(L)
      G=DIG(L)/SLG(L)
      CB=LOGF(G)
      BB=LOGF(B)
      AB=LOGF(A)
      AA=(1.5*AB)+(0.5*BB)+CB
      CAN=(PGR*AA)-17.1614
      N=NCD(I)
      DO 7542 J=1,N
      U=EWP(L,J)/THA
      EU=EXPF(U)
      EUD=EU-1.0
      EP=EU/EUD
      EH=U/EUD
      EL=LOGF(EP)
      EN=EN+EH
 7542 ENF=ENF+EL
      BNT=LOGF(TDC)
      PEK=CAN+PGR*((4.0*BNT)+ENF)
      PENT=PGR*(EN)
      GO TO 5790
C       COMPUTATION FOR  ELECTRONS AND PROTONS
 5751 PENT=(2.50*PGR)
      AB=LOGF(TDC)
      BB=LOGF(SWTM(I))
      TEE=1.0-SWTM(I)
      IF(TEE)5753,5753,5752
 5752 CB=LOGF(2.0)
      GO TO 5754
 5753 CB=0.0
 5754 PEK=PGR*((2.5*AB)+(1.5*BB)+CB)-7.28353
      GO TO 5790
 5790 RETURN
      END
      SUBROUTINE PRIN(KDT)
     0DIMENSION NA(10),SWTM(100),NPM(100),NCD(100),SEFR(100),SFORM(100),
     1STY(100,10),IDRC(100),IDRE(10),CON(100),IID(9),FR(9),CONR(9),
     2STSB(10),SY(100,10),Y(10,10),SB(100),WTM(100),EFR(100),FORM(100),
     3ENT(100),EK(100),CPP(100),PHI(100),D(100),C(100),Z(100),DSO(100),
     4CONOLD(100),DELDH(2),SFCON(100),SIG(100),ELAT(32,70),DEGE(32,70),
     5LOC(100),SLG(75),DIG(75),EBP(75),
     6EAP(75),EIP(75),EWP(75,12),ETE(20,10),EWE(20,10),
     7EWX(20,10),EBE(20,10),EAL(20,10),DEG(20,10)
      COMMON NPM, NCD,SIG,ELAT,DEGE,EWE,EWX,EBE,EAL,DEG,LOC,SLG,DIG,EBP
     1,EAP,EIP,EWP,ETE,SWTM,FORM,FR,CONR,CON,BRPT2,BRPT5,BRPT6,BRPT7,
     2BRPT8,CS2,DIN,DSAIR,DS2,ENTHA,ENTRO,HOT,PRESR,PRES1,PRES2,PRPT1,
     3RHOR,RRTT2,RRTT5,RRTT6,RRTT7,STAGE,TEMP,T1,VGAS,VRTO,WWTSTP,ZSA,
     4KIP,LARG
  300 FORMAT(1H1 9X,70H CHEMICAL EQUILIBRIUM COMPOSITION AND PROPERTIES
     1OF A COMPLEX MIXTURE /)
  301 FORMAT(1H1 9X,38H REAL GAS NORMAL SHOCK WAVE PROPERTIES /)
 3020FORMAT(1H1 9X,49H REAL GAS STANDING NORMAL SHOCK WAVE PROPERTIES
     1/)
```

```
3030FORMAT(1H1 9X,49H REAL GAS REFLECTED NORMAL SHOCK WAVE PROPERTIES
   1/)
304 FORMAT(34H  INITIAL CONDITIONS  TEMP DEG K--1E10.4,4X,8H  P/P0--
   1 1E10.4)
3050FORMAT(40H                          MOLE FRACTION OF  A6,13H AT S.T.P
   1.---1F7.5)
306 FORMAT(49H                CONCENTRATION      MOLE FRACTION )
307 FORMAT(36H           PARTICLES/CC  MOLE/LITER )
308 FORMAT(3X,A6,3E12.4)
309 FORMAT(100H                 CONCENTRATION      MOLE FRACTION
   1       CONCENTRATION      MOLE FRACTION      )
310 FORMAT(82H           PARTICLES/CC  MOLE/LITER
   1 PARTICLES/CC  MOLE/LITER )
311 FORMAT(3X,A6,3E12.4,3X,A6,3E12.4)
3120FORMAT(26H  TEMPERATURE (DEG K)-----1E11.4,14H  RHO1/RHO0---1E10.4
   1,26H  RHO0 (GM/LITER)---------1E10.4)
3130FORMAT(26H  ENTHALPY (HM0/RT0)------1E11.4,14H  P1/P0-------1E10.4
   1,26H  MIXTURE COLD MOL WT-----1E10.4)
3140FORMAT(26H  SHOCK VELOCITY (FPS)----1E11.4,14H  RHO2/RHO0-- 1E10.4
   1,26H  VEL BEHIND SHOCK (FPS)--1E10.4)
3150FORMAT(26H  TEMPERATURE (DEG K)-----1E11.4,14H  RHO2/RHO1-- 1E10.4
   1,26H  ENTROPY (SM0/R)---------1E10.4)
3160FORMAT(26H  ENTHALPY (HM0/RT0)------1E11.4,14H  P2/P0------ 1E10.4
   1,26H  Z-----------------------1E10.4)
3170FORMAT(26H  STAG ENTHALPY (HM0/RT0)-1E11.4,14H  P2/P1------ 1E10.4
   1)
318 FORMAT(22H   INITIAL CONDITIONS )
319 FORMAT(20H   FINAL CONDITIONS )
3200FORMAT(26H  SHOCK VELOCITY (FPS)----1E11.4,14H  P3/P0-------1E10.4
   1,26H  VEL BEHIND ST SHOCK-----1E10.4)
3210FORMAT(26H  TEMPERATURE (DEG K)-----1E11.4,14H  P3/P2-------1E10.4
   1,26H  STAG ENTHALPY (HM0/RT0)-1E10.4)
3220FORMAT(26H  ENTHALPY (HM0/RT0)------1E11.4,14H  RHO3/RHO0---1E10.4
   1,26H  ENTROPY (SM0/R)---------1E10.4)
3230FORMAT(26H  M0-MIXTURE COLD MOL WT--1E11.4,14H  RHO3/RHO2---1E10.4
   1,26H  Z-----------------------1E10.4)
3240FORMAT(50H                                      RHO0 (GM/L)-1E10.4
   1)
3250FORMAT(26H  SHOCK VELOCITY (FPS)----1E11.4,14H  P4/P0-------1E10.4
   1,26H  REF SHOCK VEL (FPS)-----1E10.4)
3260FORMAT(26H  TEMPERATURE (DEG K)-----1E11.4,14H  P4/P2-------1E10.4
   1,26H  ENTROPY (SM0/R)---------1E10.4)
3270FORMAT(26H  ENTHALPY (HM0/RT0)------1E11.4,14H  RHO4/RHO0---1E10.4
   1,26H  Z-----------------------1E10.4)
3280FORMAT(26H  M0-MIXTURE COLD MOL WT--1E11.4,14H  RHO4/RHO2---1E10.4
   1,26H  RHO0--------------------1E10.4)
3290FORMAT(26H  TEMPERATURE (DEG K)-----1E11.4,14H  P/P0--------1E10.4
   1,26H  ENTROPY (SM0/R)---------1E10.4)
3300FORMAT(26H  ENTHALPY (HM0/RT0)------1E11.4,14H  RHO/RHO0----1E10.4
   1,26H  RHO0--------------------1E10.4)
3310FORMAT(26H  MIXTURE COLD MOL WT-----1E11.4,14H  Z-----------1E10.4
   1/)
     GO TO(1300,1310,1320,1330),KDT
1300 WRITE OUTPUT TAPE 6,300
     WRITE OUTPUT TAPE 6,318
     GO TO 1340
1310 WRITE OUTPUT TAPE 6,301
     WRITE OUTPUT TAPE 6,318
     VPP=(DIN*WWTSTP)/28.9662
```

```
      WRITE OUTPUT TAPE 6,312,T1,VPP,DSAIR
      WRITE OUTPUT TAPE 6,313,HOT,PRES1,WWTSTP
      GO TO 1340
 1320 WRITE OUTPUT TAPE 6,302
      GO TO 1331
 1330 WRITE OUTPUT TAPE 6,303
 1331 WRITE OUTPUT TAPE 6,304,T1,PRES1
 1340 DO 1341 I=1,KIP
 1341 WRITE OUTPUT TAPE 6,305,FR(I),CONR(I)
      WRITE OUTPUT TAPE 6,319
      IF(LARG-35) 1350,1370,1370
 1350 WRITE OUTPUT TAPE 6,306
      WRITE OUTPUT TAPE 6,307
      DO 1351 I=1,LARG
      CPMOL=CON(I)*0.602338E+21
      CONFR=CON(I)/CS2
 1351 WRITE OUTPUT TAPE 6,308,FORM(I),CPMOL,CON(I),CONFR
      GO TO 1376
 1370 WRITE OUTPUT TAPE 6,309
      WRITE OUTPUT TAPE 6,310
      I=1
 1371 J=I+1
      IF(J-LARG) 1373,1374,1375
 1373 CONF1=CON(I)/CS2
      CONF2=CON(J)/CS2
      CPML1=CON(I)*0.602338E+21
      CPML2=CON(J)*0.602338E+21
      WRITE OUTPUT TAPE 6,311,FORM(I),CPML1,CON(I),CONF1,FORM(J),CPML2,
     1CON(J),CONF2
      I=I+2
      GO TO 1371
 1374 CONF1=CON(I)/CS2
      CONF2=CON(J)/CS2
      CPML1=CON(I)*0.602338E+21
      CPML2=CON(J)*0.602338E+21
      WRITE OUTPUT TAPE 6,311,FORM(I),CPML1,CON(I),CONF1,FORM(J),CPML2,
     1CON(J),CONF2
      GO TO 1376
 1375 CONF1=CON(I)/CS2
      CPML1=CON(I)*0.602338E+21
      WRITE OUTPUT TAPE 6,308,FORM(I),CPML1,CON(I),CONF1
 1376 CONTINUE
      GO TO (1380,1385,1390,1395),KDT
 1380 WRITE OUTPUT TAPE 6,329,TEMP,PRES2,ENTRO
      WRITE OUTPUT TAPE 6,330,ENTHA,VRTO,DSAIR
      WRITE OUTPUT TAPE 6,331,WWTSTP,ZSA
      GO TO 1399
 1385 VPP=DS2/DSAIR
      WRITE OUTPUT TAPE 6,314,PRPT1,VPP,VGAS
      WRITE OUTPUT TAPE 6,315,TEMP,RHOR,ENTRO
      WRITE OUTPUT TAPE 6,316,ENTHA,PRES2,ZSA
      WRITE OUTPUT TAPE 6,317,STAGE,PRESR
      GO TO 1399
 1390 WRITE OUTPUT TAPE 6,320,PRPTI,PRES2,BRPT6
      WRITE OUTPUT TAPE 6,321,TEMP,BRPT7,BRPT5
      WRITE OUTPUT TAPE 6,322,ENTHA,BRPT2,ENTRO
      WRITE OUTPUT TAPE 6,323,WWTSTP,BRPT8,ZSA
      WRITE OUTPUT TAPE 6,324,DSAIR
      GO TO 1399
 1395 WRITE OUTPUT TAPE 6,325,PRPT1,PRES2,RRTT7
      WRITE OUTPUT TAPE 6,326,TEMP,RRTT5,ENTRO
      WRITE OUTPUT TAPE 6,327,ENTHA,RRTT2,ZSA
      WRITE OUTPUT TAPE 6,328,WWTSTP,RRTT6,DSAIR
 1399 RETURN
      END
```

Nomenclature for Library Data

MAXE = Number of components required to represent the formula vectors of all chemical species considered in the library. This is the number of elements plus the electron.

MAXS = Total number of chemical species considered in the library.

NA = Temporary storage for formula vector.

SWTM = Library storage location for molecular weights.

NPM = Identification number for the different types of chemical species: (atomic and atomic ion species NPM = 01), (diatomic species NPM = 02), (linear polyatomic NPM = 03), (nonlinear polyatomic NPM = 04), (Protons, HE III, Electrons NPM = 05).

NCD = Number of data cards which make up a library packet for each specie:

(1) For atomic and atomic ion species. This is the number of energy level cards in the library and NCD $\leq$ 70.

(2) For diatomic species. This is the number of electronic energy level cards in the library and NCD $\leq$ 10.

(3) For polyatomic species. This is the number of vibrational frequencies in the library and NCD $\leq$ 12. Only ground electronic levels are considered.

SEFR = Library storage location of heats of formation (kcal/mole).

SFORM = Library storage location of chemical symbols for species.

STY = Library storage location for the components of the formula vector for each specie.

DEGE = Atomic specie degeneracy $\Sigma (2j + 1)$ for an energy level, g.

ELAT = Atomic specie energy levels, ϵ.

} 32 species; 70 levels.

LOC = Number locating energy level library data within the respective blocks for atomic, diatomic and polyatomic species.

ETE = Diatomic T_e, electronic term values

EWE = Diatomic ω_e

EWX = Diatomic $\omega_e x_e$ } vibrational parameters

EBE = Diatomic B_e

EAL = Diatomic α_e } rotational parameters

DEG = Diatomic p, degeneracy

SIG = Diatomic σ symmetry parameter

} Dimensioned for a maximum of 20 species with 10 electronic levels.

Nomenclature for Library Data (contd)

SLG = Linear and nonlinear polyatomic σ symmetry parameter

DIG = Linear and nonlinear polyatomic p degeneracy

EBP = Linear polyatomic Be

EAP = Linear polyatomic α_e

} rotational parameters

EIP = Nonlinear polyatomic $I_A \times I_B \times I_C$ product of moments of inertia

EWP = Nonlinear and linear polyatomic ω

} Dimensions for 75 polyatomic species with a max of 12 vibration frequencies each.

Nomenclature for Case Input

LARG = Total number of species in the high temperature case under consideration.

MIN = Total number of formula vector components required to represent the species in the high temperature mixture; the number of elements plus the electron.

IDRC = Identification number used to select the high temperature product species from the library list.

IDRE = Identification number used to select the high temperature components (electrons plus elements) from the library list.

CON = Storage locations of the high temperature species concentrations.

ITER = Number of iterations through the equilibrium block (i.e., mass action and mass balance equations).

KIT = A number which is "1" when externally supplied initial guesses of component concentrations are used to start the computation. For all successive computations in which the concentrations from the previous solution are used to start the concentration computation, the value is "2."

Nomenclature for Case Input (contd)

IST = Case control number:

(1) IST = 00; Equilibrium solution or Mollier data case

(2) IST = 01; Moving shock case

(3) IST = 02; Combination moving, standing, and reflected cases

(4) IST = 03; Combination of moving and standing cases

(5) IST = 04; Combination of moving and reflected cases

KIP = Number of species in the initial or STP mixture.

IID = Identification number used to select the reactants data from the library list.

FR = Chemical symbol for reactant.

CONR = Fraction of reactant in mixture at STP.

STSB = B_i—concentration of the ith element at STP, moles/liter.

SY = Storage location of modified formula vector used in the case computation.

SB = Concentration "*STSB*" or B_i used in the case computation.

WTM = Storage location of molecular weights used in the case computation.

EFR = Storage location of heat of formation used in the case computation.

FORM = Storage location of chemical symbol used in the case computation.

ENT = Computed $(H - H_o^o)/T$.

EK = Computed $-(F - H_o^o)/T$.

CPP = H, cal/mole.

PHI = Computed equilibrium constant.

TEMP = Equilibrium temperature, °K.

HGP = Initial pressure P_1 in atmospheres (atm).

T1 = Initial temperature, T_1 in °K.

VRTO = Equilibrium density ratio, ρ/ρ_o.

Appendix E

Library Data

```
0866
1           C2      2 0 0 0 0 0 0 0 0 0 0 24.07230 02    9 2.0
 C2  HEAT FORMATION 0.196000E 03
C2     LC A SINGLET SIGMA        0.0     1854.7     13.34      1.820     0.01760    1.0
C2     X TRIPLET SIGMA         716.2     1641.3     11.67      1.633     0.01640    6.0
C2     TRIPLET PI             6435.1     1470.4     11.19      1.499     0.01630    3.0
C2     LC B SINGLET PI        8391.1     1608.3     12.08      1.616     0.01690    2.0
C2     SINGLET DELTA         10186.3     1481.0     11.14      1.486     0.01500    2.0
C2     SINGLET SIGMA         14191.5     1470.0     10.06      1.475     0.013      1.0
C2     TRIPLET SIGMA         14282.1     1891.0     14.23      1.897     0.01800    3.0
C2     A TRIPLET PI          19950.3     1788.2     16.44      1.753     0.0161     6.0
C2     C SINGLET PI          34277.4     1809.1     15.81      1.733     0.018      2.0
2           N2      0 2 0 0 0 0 0 0 0 0 0 28.01340 02    2 2.0
 N2  HEAT FORMATION 0.       E 00
N2     X SINGLET SIGMA           0.0     2358.1     14.19      1.990     0.0170     1.0
N2     A TRIPLET SIGMA       50206.0     1460.4     13.89      1.430     0.0130     3.0
3           O2      0 0 2 0 0 0 0 0 0 0 0 31.99880 02    4 2.0
 O2  HEAT FORMATION 0.       E 00
O2     X TRIPLET SIGMA           0.0     1580.4     12.07      1.446     0.0158     3.0
O2     LC A SINGLET DELTA     7918.1     1509.0     12.00      1.426     0.0171     2.0
O2     LC B SIGMA            13195.2     1432.7     13.95      1.400     0.0182     1.0
O2     A TRIPLET SIGMA       36096.0      819.0     22.50      1.050                3.0
4           H2      0 0 0 2 0 0 0 0 0 0  2.01594 02    1 2.0
H2  HEAT FORMATION   .000000E 00
H2     X SINGLET SIGMA           0.0     4395.2    117.9      60.81      2.99000    1.0
5           CN      1 1 0 0 0 0 0 0 0 0 26.01785 02    3 1.0
 CN  HEAT FORMATION 0.109000E 03
CN     X DOUBLET SIGMA           0.0     2068.8     13.19      1.900     0.0180     2.0
CN     A DOUBLET PI           9246.0     1812.6     12.70      1.720     0.0170     4.0
CN     B DOUBLET SIGMA       25752.1     2163.7     20.10      1.970     0.0220     2.0
6           CO      1 0 1 0 0 0 0 0 0 0 28.01055 02    2 1.0
 CO  HEAT FORMATION -.271990E 02
CO     X SINGLET SIGMA           0.0     2169.8     13.29      1.931     0.0175     1.0
CO     LC A TRIPLET PI       48687.4     1743.6     14.47      1.691     0.0195     6.0
7           CH      1 0 0 1 0 0 0 0 0 0 13.01912 02    5 1.0
CH  HEAT FORMATION   .141600E 03
CH     X DOUBLET PI              0.0     2861.6     64.30     14.460     0.53400    2.0
CH     X DOUBLET PI             17.9     2861.6     64.30     14.460     0.53400    2.0
CH     A DOUBLET DELTA       23150.0     2921.0     90.40     14.910     0.67000    4.0
CH     B DOUBLET SIGMA       25993.0     1808.0    201.50      7.170     0.53000    2.0
CH     C DOUBLET SIGMA       31828.0     2073.4     57.00      7.880     0.28000    2.0
8           NO      0 1 1 0 0 0 0 0 0 0 30.00610 02    4 1.0
 NO  HEAT FORMATION 0.214500E 02
NO     X DOUBLET PI              0.0     1903.7     13.97      1.705     0.0178     2.0
NO     X DOUBLET PI            121.1     1903.4     13.97      1.705     0.0178     2.0
NO     LC A QUAD PI          38406.0     1019.0     12.80      1.220     0.0198     8.0
NO     A DOUBLET SIGMA       43966.0     2371.0     14.50      1.995     0.0164     2.0
9           NH      0 1 0 1 0 0 0 0 0 0 15.01467 02    4 1.0
NH   HEAT FORMATION +.790000E+02
NH     X TRIPLET SIGMA           0.0     3315.0     94.7       16.67      0.65       3.0
NH     LC A SINGLET DELTA    14970.0     3186.0     29.0       16.54      0.17       2.0
NH     LC B SINGLET SIGMA    23415.0     3480.0                16.40                 1.0
NH     A TRIPLET PI          29819.0     3232.5     99.2       16.69      0.74       6.0
10          OH      0 0 1 1 0 0 0 0 0 0 17.00737 02    2 1.0
OH  HEAT FORMATION   .925000E 01
OH     X DOUBLET PI              0.0     3738.4     81.80      18.850     0.70000    4.0
OH     A DOUBLET SIGMA       32687.0     3179.4    103.30      17.230     0.78000    2.0
11          CO+     1 0 1 0 0 0 0-1 0 0 28.01000 02    3 1.0
 CO+ HEAT FORMATION 0.295900E 03
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CO+    X DOUBLET SIGMA          0.0     2214.3     15.16      1.977     0.0190     2.0
CO+    A DOUBLET PI         20733.0     1562.1     13.53      1.589     0.01940    4.0
CO+    B DOUBLET SIGMA      45877.0     1734.2     27.93      1.800     0.03020    2.0
12           CH+     1 0 0 1 0 0 0-1 0 0 13.01857 02    2 0.0
CH+   HEAT FORMATION +.398100E+03
CH+    X SINGLET SIGMA          0.0     2739.7               14.18      0.49       1.0
CH+    A SINGLET PI         24171.3     1840.1     98.5      11.89      0.92       2.0
13           N2+     0 2 0 0 0 0 0-1 0 0 28.01285 02    3 2.0
 N2+  HEAT FORMATION 0.359297E 03
N2+    X DOUBLET SIGMA          0.0     2207.6     16.90      1.9300    0.02000    2.0
N2+    A DOUBLET PI          9168.3     1902.8     14.60      1.7400    0.01800    4.0
N2+    B DOUBLET SIGMA      25452.9     2441.1     31.20      2.0850    0.02500    2.0
14           NO-     0 1 1 0 0 0 0 1 0 0 30.00665 02    1 1.0
NO-   HEAT FORMATION +.140000E+02
NO-    TRIPLET SIGMA            0.0     1600.0     12.0       1.4       0.016      3.0
15           NO+     0 1 1 0 0 0 0-1 0 0 30.008   02    2 1.0
NO+  HEAT FORMATION   .235170E 03
NO+    X SINGLET SIGMA          0.0     2377.1     16.35      2.0020    0.02020    1.0
NO+    LC A TRIPLET SIGMA   40332.0     1572.0                                     3.0
16           O2+     0 0 2 0 0 0 0-1 0 0 31.99825 02    4 2.0
 O2+  HEAT FORMATION 0.278178E+03
O2+    X DOUBLET PI             0.0     1876.4     16.53      1.6722    0.01984    2.0
O2+    X DOUBLET PI           200.0     1876.4     16.53      1.6722    0.01984    2.0
O2+    LC,A QUAD PI         31900.0     1035.7     10.39      1.1047    0.01575    8.0
O2+    A DOUBLET PI         38795.0      900.0     13.40      1.0617    0.01906    4.0
17           O2-     0 0 2 0 0 0 0 1 0 0 31.99935 02    2 2.0
 O2-  HEAT FORMATION -.133700E 02
O2-    DOUBLET PI LC G          0.0     1170.0      8.50      1.247     0.0130     4.0
O2-    DOUBLET PI LC U      29400.0                                                4.0
18           OH+     0 0 1 1 0 0 0-1 0 0 17.00682 02    2 1.0
OH+   HEAT FORMATION +.316000E+03
OH+    X TRIPLET SIGMA          0.0     3229.0    131.0      16.74     0.73       3.0
OH+    TRIPLET PI           28459.0     2202.0    108.0      13.75     0.86       6.0
19           OH-     0 0 1 1 0 0 0 1 0 0 17.00792 02    1 1.0
OH-   HEAT FORMATION -.329000E+02
OH-    X SINGLET SIGMA          0.0     3735.0     74.7      18.87     0.65       1.0
20           H2+     0 0 0 2 0 0 0-1 0 0  2.01539 02    1 2.0
H2+   HEAT FORMATION +.355740E+03
H2+    X DOUBLET SIGMA          0.0     2297.0     62.0      29.80     1.4        2.0
21           C3      3 0 0 0 0 0 0 0 0 0 36.03345 03    4 0.0
C3   HEAT FORMATION  0.188000E+03
C3     SINGLET SIGMA       2.01.0 0.4280  0.0      4
  500.0
  500.0
 1300.0
 2200.0
22           C2N2    2 2 0 0 0 0 0 0 0 0 0 52.03570 03    7 0.0
C2N2HEAT FORMATION  0.734000E+02
C2N2   SINGLET SIGMA       2.01.0 0.1605  0.0      7
  226.0
  226.0
  506.0
  506.0
  848.0
 2149.0
 2322.0
23           CO2     1 0 2 0 0 0 0 0 0 0 44.00995 03    4 0.0
CO2   HEAT FORMATION -.939630E+02
CO2    SINGLET SIGMA       2.01.0 0.39021 0.0022   4
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 1388.17
  667.40
  667.40
 2349.16
24          C2H    2 0 0 1 0 0 0 0 0 0 25.03027 03    4 0.0
 C2H HEAT FORMATION  .116700E+03
C2H   DOUBLET PI          1.04.0 1.4482  0.0      4
 1923.4
 3216.7
  712.0
  712.0
25          C2H2   2 0 0 2 0 0 0 0 0 0 26.03824 03    7 0.0
 C2H2HEAT FORMATION  .543300E+02
C2H2  SINGLET SIGMA       2.01.0 1.17649 0.0      7
 3372.0
 1973.0
 3288.0
  729.0
  729.0
  612.0
  612.0
26          N2O    0 2 1 0 0 0 0 0 0 0 44.01280 03    4 0.0
N2O  HEAT FORMATION +.204350E+02
N2O   SINGLET SIGMA       1.01.0 0.41901 0.0040   4
 2223.7
  588.8
  588.8
 1284.9
27          CH2    1 0 0 2 0 0 0 0 0 0 14.02709 04    3 0.0
 CH2 HEAT FORMATION  .950000E+02
CH2   SINGLET A           2.01.0 1.39300E-40 2.57100E-40 3.96400E-4003
CH2   SINGLET A            3105.0
CH2   SINGLET A            3019.0
CH2   SINGLET A            1570.0
28          CH3    1 0 0 3 0 0 0 0 0 0 15.03506 04    6 0.0
 CH3 HEAT FORMATION  .334000E+02
CH3   DOUBLET A           6.02.0 5.85500E-40 2.92800E-40 2.92800E-4006
CH3   DOUBLET A            2920.0
CH3   DOUBLET A             447.0
CH3   DOUBLET A            1228.0
CH3   DOUBLET A            1228.0
CH3   DOUBLET A            3000.0
CH3   DOUBLET A            3000.0
29          CH4    1 0 0 4 0 0 0 0 0 0 16.04303 04    9 0.0
 CH4 HEAT FORMATION -.159900E+02
CH4   SINGLET A          12.01.0 5.33000E-40 5.33000E-40 5.33000E-4009
CH4   SINGLET A            2914.2
CH4   SINGLET A            1526.0
CH4   SINGLET A            1526.0
CH4   SINGLET A            1300.2
CH4   SINGLET A            1300.2
CH4   SINGLET A            1300.2
CH4   SINGLET A            3020.3
CH4   SINGLET A            3020.3
CH4   SINGLET A            3020.3
30          CHO+   1 0 1 1 0 0 0-1 0 0 29.01797 04    3 0.0
 CHO+HEAT FORMATION  .205000E+03
CHO+  SIGMA               1.02.018.72920E-4012.51470E-4019.92120E-4003
CHO+  SIGMA                2700.0
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CHO+  SIGMA                1820.2
CHO+  SIGMA                1083.0
31          CH2O   1 0 1 2 0 0 0 0 0 0 0 30.02649 04   6 0.0
 CH2OHEAT FORMATION -.269000E+02
CH2O  SIGMA               2.01.0 2.97500E-4021.60800E-4024.67000E-4006
CH2O  SIGMA                2780.0
CH2O  SIGMA                2843.0
CH2O  SIGMA                1746.0
CH2O  SIGMA                1247.0
CH2O  SIGMA                1500.0
CH2O  SIGMA                1167.0
32          NO2    0 1 2 0 0 0 0 0 0 0 0 46.00550 04   3 0.0
NO2  HEAT FORMATION +.860000E+01
NO2                       2.02.068.20000E-4064.55000E-40 3.48600E-40
NO2                        1319.7
NO2                         749.8
NO2                        1617.75
33          NH3    0 1 0 3 0 0 0 0 0 0 0 17.03061 04   6 0.0
NH3  HEAT FORMATION -.934000E+01
NH3                       3.01.0 2.81400E-40 2.81400E-40 4.51730E-40
NH3                        3336.2
NH3                         949.87
NH3                        3443.9
NH3                        3443.6
NH3                        1627.4
NH3                        1626.1
34          O3     0 0 3 0 0 0 0 0 0 0 0 47.99820 04   3 0.0
O3  HEAT FORMATION  0.346390E+02
O3                        2.01.0 7.87490E-4062.84400E-4070.88800E-4003
O3                          705.0
O3                         1043.0
O3                         1110.0
35          H2O    0 0 1 2 0 0 0 0 0 0 0 18.01534 04   3 0.0
H2O  HEAT FORMATION -.571020E+02
H2O   SINGLET SIGMA       2.01.0 1.00400E-40 1.92900E-40 3.01500E-4003
H2O                        3657.0
H2O                        1594.7
H2O                        3755.7
36          HCO    1 0 1 1 0 0 0 0 0 0 0 29.01852 04   3 0.0
 HCO HEAT FORMATION  .000000E+00
HCO   DOUBLET A           1.02.018.72920E-40 1.25147E-4019.92120E-4003
HCO   DOUBLET A            2700.0
HCO   DOUBLET A            1820.2
HCO   DOUBLET A            1083.0
37          C-     1 0 0 0 0 0 0 1 0 0 12.01170 01  51 0.0
C-   HEAT FORMATION  .144000E 03
  C-                  4.00          0.0
  C-                 10.00      19223.000
  C-                  6.00      28840.000
  C-                 12.00      83366.000
  C-                  6.00      86223.187
  C-                 12.00      88109.500
  C-                  2.00      93582.250
  C-                 20.00      94883.062
  C-                 12.00      95533.187
  C-                 14.00      96864.187
  C-                  6.00      97805.750
  C-                 10.00      99665.000
  C-                 12.00     103736.750
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 C-                  6.00    104227.375
 C-                 34.00    104767.000
 C-                 32.00    104882.687
 C-                 24.00    105020.000
 C-                  2.00    106478.562
 C-                  6.00    106780.062
 C-                 20.00    106870.687
 C-                 10.00    107039.000
 C-                 12.00    109927.875
 C-                  2.00    110029.187
 C-                  8.00    110196.000
 C-                 32.00    110248.000
 C-                 38.00    110304.000
 C-                 16.00    110470.500
 C-                 10.00    110545.750
 C-                  6.00    112320.750
 C-                  2.00    112565.875
 C-                 10.00    112682.562
 C-                 20.00    112799.000
 C-                 60.00    112862.000
 C-                 16.00    112947.500
 C-                  6.00    114072.000
 C-                 62.00    114160.000
 C-                 40.00    114275.000
 C-                  6.00    114890.000
 C-                 32.00    114988.000
 C-                 24.00    115004.000
 C-                 18.00    115103.000
 C-                 18.00    115483.000
 C-                 44.00    115535.000
 C-                 18.00    115618.000
 C-                 44.00    115887.000
 C-                 36.00    115902.000
 C-                 58.00    116164.000
 C-                 22.00    116259.000
 C-                 58.00    116367.000
 C-                 28.00    116441.000
 C-                 28.00    116625.000
38          C+     1 0 0 0 0 0 0-1 0 0 12.0106  01  36 0.0
 C+  HEAT FORMATION 0.429537E 03
 CII                 2.00        0.0
 CII                 4.00       64.000
 CII                 2.00    43000.199
 CII                 4.00    43021.797
 CII                 6.00    43050.699
 CII                 6.00    74930.875
 CII                 4.00    74933.187
 CII                 2.00    96494.062
 CII                 6.00   110666.250
 CII                 2.00   116537.875
 CII                 6.00   131735.750
 CII                 4.00   142024.375
 CII                10.00   145551.437
 CII                10.00   150462.750
 CII                 2.00   157234.375
 CII                 6.00   162524.562
 CII                 6.00   166988.437
 CII                 6.00   167033.375
 CII                16.00   168124.312
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  CII                14.00    168979.000
  CII                 2.00    173348.125
  CII                 6.00    175295.187
  CII                 6.00    178220.750
  CII                10.00    178494.750
  CII                14.00    178956.437
  CII                 2.00    181258.000
  CII                20.00    181770.437
  CII                 6.00    182044.500
  CII                10.00    184064.875
  CII                14.00    184376.187
  CII                 4.00    184688.687
  CII                12.00    186463.750
  CII                10.00    188612.687
  CII                 2.00    194571.875
  CII                28.00    195812.250
  CII                20.00    196580.750
39          C++    1 0 0 0 0 0 0-2 0 0 12.01005 01  20 0.0
 C++ HEAT FORMATION 0.991689E 03
  CIII               1.00        0.0
  CIII               5.00     52394.797
  CIII               4.00     52338.000
  CIII               3.00    102351.375
  CIII               9.00    137450.500
  CIII               5.00    145875.062
  CIII               1.00    182520.187
  CIII               4.00    238160.687
  CIII              12.00    259672.062
  CIII              15.00    269962.875
  CIII               5.00    276482.687
  CIII              12.00    308264.750
  CIII              16.00    317748.000
  CIII              78.00    321964.687
  CIII              49.00    333395.000
  CIII             116.00    346526.000
  CIII              90.00    358639.000
  CIII              29.00    365585.000
  CIII              39.00    373748.000
  CIII              37.00    381958.000
40          C+++   1 0 0 0 0 0 0-3 0 0 12.0095  01  22 0.0
 C+++HEAT FORMATION 0.209569E 04
  CIV                2.00        0.0
  CIV                2.00     64484.199
  CIV                4.00     64591.297
  CIV                2.00    302847.875
  CIV                6.00    320080.000
  CIV               10.00    324890.875
  CIV                2.00    401346.687
  CIV                6.00    408322.187
  CIV               10.00    410338.187
  CIV               14.00    410434.062
  CIV                2.00    445366.062
  CIV                6.00    448861.000
  CIV               42.00    449948.375
  CIV                2.00    468765.000
  CIV                6.00    470763.000
  CIV               64.00    471407.875
  CIV                2.00    482659.000
  CIV                6.00    483931.000
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  CIV                10.00    484309.000
  CIV                54.00    484346.875
  CIV                20.00    492743.000
  CIV                60.00    492745.000
41          N-      0 1 0 0 0 0 0 1 0 0 14.00725 01  32 0.0
N-   HEAT FORMATION  .115990E 03
  N-                 5.00         0.0
  N-                 3.00       158.500
  N-                 1.00       226.500
  N-                 5.00     15867.699
  N-                 1.00     33792.398
  N-                 5.00     73767.750
  N-                 3.00     76794.687
  N-                15.00     86631.000
  N-                 9.00     88630.812
  N-                 5.00     95476.375
  N-                 3.00     96225.500
  N-                45.00     97420.187
  N-                15.00     99094.500
  N-                 9.00     99680.375
  N-                15.00    101135.000
  N-                 5.00    102116.187
  N-                 3.00    102411.625
  N-                 5.00    102661.625
  N-                25.00    102865.062
  N-                15.00    102908.125
  N-                 9.00    103869.375
  N-                 8.00    105019.000
  N-                40.00    105385.250
  N-                 9.00    105911.250
  N-                 8.00    106545.062
  N-                40.00    106751.187
  N-                 8.00    107445.375
  N-                40.00    107573.062
  N-                 8.00    108021.375
  N-                40.00    108105.687
  N-                48.00    108470.187
  N-                48.00    108731.500
42          N+      0 1 0 0 0 0 0-1 0 0 14.00615 01  54 0.0
 N+  HEAT FORMATION 0.447564E 03
   NII               1.00         0.0
   NII               3.00        49.100
   NII               5.00       131.300
   NII               5.00     15315.699
   NII               1.00     32687.098
   NII               5.00     47167.699
   NII              15.00     92237.875
   NII               9.00    109218.187
   NII               5.00    144189.062
   NII              12.00    149077.312
   NII               3.00    155129.875
   NII               3.00    164611.562
   NII              15.00    166679.437
   NII               3.00    166765.687
   NII               3.00    168893.000
   NII               9.00    170667.000
   NII               6.00    174212.875
   NII              21.00    186653.312
   NII               5.00    187092.187
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   NII              15.00   187492.687
   NII               9.00   188858.062
   NII               7.00   189336.000
   NII               3.00   190121.125
   NII              21.00   209825.250
   NII               5.00   209926.875
   NII              15.00   210301.875
   NII               9.00   210705.375
   NII               7.00   211104.750
   NII               3.00   211335.500
   NII              15.00   220717.000
   NII               7.00   221137.562
   NII              15.00   206108.687
   NII               9.00   211828.750
   NII               9.00   196712.125
   NII               3.00   197859.250
   NII               9.00   214385.250
   NII               3.00   214828.000
   NII              25.00   224169.250
   NII              20.00   226055.187
   NII               3.00   202169.875
   NII              15.00   202862.000
   NII               9.00   203259.687
   NII               3.00   203532.750
   NII               5.00   205350.687
   NII               1.00   206327.500
   NII               7.00   211030.875
   NII              21.00   211061.000
   NII              27.00   211390.750
   NII               9.00   211402.875
   NII              15.00   211411.250
   NII               5.00   211491.125
   NII              21.00   221074.250
   NII              27.00   221302.187
   NII               9.00   221312.062
43          N++    0 1 0 0 0 0 0-2 0 0 14.00560 01  43 0.0
 N++ HEAT FORMATION 0.113022E 04
  NIII              2.00       0.0
  NIII              4.00     174.500
  NIII              2.00   57192.098
  NIII              4.00   57252.000
  NIII              6.00   57333.199
  NIII             10.00  101023.750
  NIII              2.00  131003.500
  NIII              2.00  145876.062
  NIII              4.00  145986.500
  NIII              4.00  186802.250
  NIII             10.00  203072.187
  NIII              2.00  221302.375
  NIII              6.00  230408.562
  NIII              6.00  245701.687
  NIII             10.00  267244.375
  NIII             12.00  287713.875
  NIII              6.00  297263.062
  NIII              2.00  301088.187
  NIII             26.00  309856.687
  NIII              6.00  311716.062
  NIII              4.00  314224.000
  NIII             12.00  317402.250
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  NIII                10.00    317781.750
  NIII                14.00    320287.500
  NIII                10.00    321065.750
  NIII                 2.00    327056.750
  NIII                28.00    330396.687
  NIII                20.00    332860.000
  NIII                12.00    334568.875
  NIII                12.00    336213.375
  NIII                14.00    339855.687
  NIII                10.00    341947.875
  NIII                20.00    342752.000
  NIII                18.00    343116.000
  NIII                10.00    354517.000
  NIII                14.00    354955.687
  NIII                18.00    355214.000
  NIII                12.00    368704.750
  NIII                10.00    373376.000
  NIII                 6.00    374805.250
  NIII                20.00    376953.250
  NIII                16.00    377970.750
  NIII                16.00    379405.000
44          N+++    0 1 0 0 0 0 0-3 0 0 14.00505 01  23 0.0
N+++ HEAT FORMATION 0.222425E 04
  NIV                 1.00         0.0
  NIV                 4.00     67199.562
  NIV                 5.00     67343.750
  NIV                 3.00    130695.000
  NIV                 4.00    175536.687
  NIV                 5.00    175661.500
  NIV                 5.00    188885.000
  NIV                 1.00    235370.000
  NIV                 3.00    377206.000
  NIV                 1.00    388858.000
  NIV                12.00    405944.375
  NIV                15.00    419979.375
  NIV                 5.00    429158.000
  NIV                 9.00    465463.375
  NIV                 3.00    473032.000
  NIV                21.00    484525.000
  NIV                40.00    499851.000
  NIV                34.00    506292.000
  NIV                53.00    516650.000
  NIV                 7.00    521868.000
  NIV                45.00    554419.000
  NIV                15.00    574940.000
  NIV                20.00    593704.000
45          O-      0 0 1 0 0 0 0 1 0 0 15.99995 01  24 0.0
O-   HEAT FORMATION  .252000E 02
 O-                  4.00         0.0
 O-                  2.00       404.000
 O-                  6.00    102406.500
 O-                  4.00    102681.240
 O-                  2.00    102841.200
 O-                  4.00    104731.860
 O-                  2.00    105057.100
 O-                  6.00    115918.700
 O-                  4.00    116041.690
 O-                  2.00    116144.390
 O-                  8.00    116988.210
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 O-                    6.00    117164.830
 O-                    6.00    117310.000
 O-                   10.00    128219.920
 O-                   22.00    128516.000
 O-                    6.00    132596.260
 O-                    4.00    132745.770
 O-                    6.00    133000.000
 O-                    2.00    133224.100
 O-                   18.00    133546.000
 O-                   10.00    133606.390
 O-                   18.00    133924.000
 O-                   14.00    137603.000
 O-                   10.00    138708.000
46          O+     0 0 1 0 0 0 0-1 0 0 15.99885 01  41 0.0
 O+  HEAT FORMATION 0.372942E 03
  OII                 4.00         0.0
  OII                10.00     26808.398
  OII                 6.00     40466.898
  OII                 6.00    119837.687
  OII                 6.00    120001.062
  OII                10.00    165987.687
  OII                 6.00    185340.625
  OII                 6.00    185499.187
  OII                 2.00    188888.375
  OII                 4.00    189068.312
  OII                 2.00    195710.375
  OII                 2.00    203942.187
  OII                30.00    207002.500
  OII                12.00    208484.187
  OII                10.00    211712.625
  OII                10.00    212593.187
  OII                 6.00    214229.437
  OII                26.00    228746.875
  OII                28.00    231530.250
  OII                52.00    232959.250
  OII                 6.00    233430.062
  OII                10.00    234454.437
  OII                12.00    238892.937
  OII                 6.00    240516.250
  OII                26.00    246028.937
  OII                16.00    248185.250
  OII                 6.00    250251.000
  OII                14.00    251220.875
  OII                18.00    252607.687
  OII                16.00    253048.312
  OII                52.00    254590.687
  OII               128.00    255977.500
  OII                42.00    256136.187
  OII                28.00    259286.187
  OII                42.00    261180.000
  OII               172.00    265925.000
  OII                18.00    267783.375
  OII                24.00    274782.375
  OII                50.00    275841.250
  OII                38.00    276109.062
  OII                10.00    278140.000
47          O++    0 0 1 0 0 0 0-2 0 0 15.99830 01  25 0.0
 O++ HEAT FORMATION 0.118260E 04
  OIII                1.00         0.0
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  OIII                3.00       113.400
  OIII                5.00       306.800
  OIII                5.00     20271.000
  OIII                1.00     43183.500
  OIII                5.00     60312.098
  OIII               15.00    120025.375
  OIII                9.00    142381.687
  OIII                8.00    187049.375
  OIII                3.00    210458.500
  OIII                9.00    267632.562
  OIII                3.00    273080.062
  OIII                9.00    283758.875
  OIII               26.00    294221.625
  OIII               14.00    306584.750
  OIII               51.00    324836.375
  OIII               25.00    338851.500
  OIII               22.00    357111.000
  OIII               64.00    365846.437
  OIII               85.00    377375.000
  OIII               19.00    380782.000
  OIII              102.00    394780.437
  OIII               96.00    401530.000
  OIII               54.00    428769.000
  OIII               61.00    438517.500
48          O+++    0 0 1 0 0 0 0-3 0 0 15.99775 01  30 0.0
 O+++HEAT FORMATION 0.244947E 04
  OIV                2.00         0.0
  OIV                4.00       386.500
  OIV                2.00     71177.000
  OIV                4.00     71308.375
  OIV                6.00     71492.875
  OIV               10.00    126936.250
  OIV                2.00    164366.875
  OIV                2.00    180481.250
  OIV                4.00    180724.562
  OIV                4.00    231275.062
  OIV               10.00    255156.687
  OIV                6.00    289024.000
  OIV                2.00    357614.750
  OIV                6.00    390248.187
  OIV               10.00    419550.187
  OIV               12.00    438970.500
  OIV                6.00    453073.000
  OIV               26.00    468499.375
  OIV               16.00    478811.250
  OIV               12.00    482923.062
  OIV               50.00    495252.750
  OIV               22.00    503834.500
  OIV               36.00    510978.500
  OIV               18.00    547336.000
  OIV               26.00    552490.000
  OIV               12.00    569020.000
  OIV               58.00    570791.000
  OIV               30.00    587850.000
  OIV              104.00    597352.000
  OIV               56.00    602977.000
49            H-    0 0 0 1 0 0 0 1 0 0  1.00852 01  16 0.0
H-    HEAT FORMATION  .344000E 02
  H-                 1.00         0.0
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  H-                  3.00    159850.312
  H-                  1.00    166271.687
  H-                 12.00    169081.062
  H-                  3.00    183231.062
  H-                  1.00    184859.000
  H-                  9.00    185558.875
  H-                 23.00    186095.875
  H-                  4.00    190292.437
  H-                 60.00    191446.562
  H-                 13.00    193795.062
  H-                 51.00    193915.750
  H-                 68.00    195256.812
  H-                188.00    196950.312
  H-                340.00    197398.562
  H-                 78.00    198056.500
50          H+     0 0 0 1 0 0 0-1 0 0  1.00742 05    0 0.0
H+  HEAT FORMATION    .365030E 03
51          AR+    0 0 0 0 1 0 0-1 0 0 39.94745 01   28 0.0
 A+ HEAT FORMATION  0.363345E 03
  AII                4.00         0.0
  AII                2.00      1433.090
  AII                2.00    108809.062
  AII               26.00    132432.125
  AII                6.00    135198.250
  AII                6.00    138353.500
  AII               18.00    142301.125
  AII               10.00    143225.437
  AII                6.00    145783.062
  AII               12.00    147993.187
  AII               18.00    149299.750
  AII               16.00    151211.000
  AII               12.00    155165.562
  AII               14.00    157361.750
  AII               12.00    158856.000
  AII                6.00    159523.187
  AII                4.00    160371.125
  AII                6.00    161177.312
  AII                2.00    167439.250
  AII               14.00    170664.062
  AII               16.00    172471.062
  AII               10.00    173534.375
  AII                6.00    174549.062
  AII               12.00    181742.312
  AII               24.00    183820.375
  AII               10.00    184133.125
  AII               18.00    185238.187
  AII               32.00    187038.250
52          AR++   0 0 0 0 1 0 0-2 0 0 39.94690 01   41 0.0
 A++HEAT FORMATION  0.100028E 04
  AIII               5.00         0.0
  AIII               3.00      1112.400
  AIII               1.00      1570.200
  AIII               5.00     14010.000
  AIII               1.00     33267.000
  AIII               5.00    113800.687
  AIII               3.00    114797.562
  AIII               1.00    115328.375
  AIII               3.00    144023.000
  AIII              25.00    144907.000
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  AIII                15.00    156917.562
  AIII                 5.00    174375.000
  AIII                 3.00    180679.000
  AIII                 9.00    186402.125
  AIII                12.00    186657.187
  AIII                 8.00    187823.000
  AIII                16.00    188714.000
  AIII                15.00    196679.750
  AIII                18.00    204797.312
  AIII                 9.00    207233.062
  AIII                 9.00    209151.812
  AIII                 7.00    210212.250
  AIII                 8.00    211004.812
  AIII                 9.00    213950.812
  AIII                15.00    225402.562
  AIII                21.00    226646.000
  AIII                 9.00    231341.750
  AIII                18.00    240291.625
  AIII                 9.00    243424.937
  AIII                25.00    246046.562
  AIII                 5.00    250712.250
  AIII                18.00    252289.000
  AIII                12.00    266877.500
  AIII                36.00    267895.812
  AIII                15.00    269000.750
  AIII                 9.00    271507.875
  AIII                18.00    272250.875
  AIII                22.00    281473.812
  AIII                 8.00    282099.125
  AIII                15.00    283919.750
  AIII                 9.00    286009.187
53          AR+++  0 0 0 0 1 0 0-3 0 0 39.94635 01  27 0.0
 A+++HEAT FORMATION 0.194349E 04
  ARIV                 4.00        0.0
  ARIV                 4.00    21090.000
  ARIV                 6.00    21219.000
  ARIV                 2.00    34854.000
  ARIV                 4.00    35035.000
  ARIV                 6.00   117564.000
  ARIV                 4.00   118515.000
  ARIV                 2.00   119044.000
  ARIV                10.00   146000.000
  ARIV                 4.00   166356.000
  ARIV                 2.00   167444.000
  ARIV                 2.00   177833.000
  ARIV                 6.00   250906.562
  ARIV                 6.00   251972.000
  ARIV                 2.00   256093.250
  ARIV                 4.00   257348.875
  ARIV                10.00   268151.375
  ARIV                 2.00   285960.125
  ARIV                10.00   286751.625
  ARIV                 8.00   287555.812
  ARIV                12.00   289834.625
  ARIV                 4.00   290256.437
  ARIV                10.00   291667.687
  ARIV                 6.00   295806.750
  ARIV                 2.00   299563.187
  ARIV                14.00   304399.875
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  ARIV                10.00    306236.250
54          NE+     0 0 0 0 0 1 0-1 0 0 20.18245 01  26 0.0
NE+ HEAT FORMATION    .497186E 03
  NEII                4.00          0.0
  NEII                2.00        782.000
  NEII                2.00     217050.000
  NEII                6.00     219133.000
  NEII                4.00     219650.750
  NEII                2.00     219949.875
  NEII                6.00     224089.250
  NEII               22.00     246396.500
  NEII               20.00     249110.750
  NEII               10.00     251013.250
  NEII                6.00     252956.000
  NEII                6.00     254167.000
  NEII               14.00     274411.250
  NEII                8.00     276278.562
  NEII               10.00     277346.062
  NEII               20.00     279139.062
  NEII               52.00     280174.375
  NEII               18.00     281173.500
  NEII               12.00     282000.000
  NEII                6.00     283323.687
  NEII               46.00     302905.750
  NEII               64.00     303475.687
  NEII               30.00     305366.187
  NEII               20.00     306689.750
  NEII               16.00     307992.187
  NEII               10.00     327954.687
55          NE++    0 0 0 0 0 1 0-2 0 0 20.18190 01  25 0.0
NE++   HEAT FORM      .144435E 04
  NEIII               5.00          0.0
  NEIII               3.00        650.000
  NEIII               1.00        927.000
  NEIII               5.00      25841.000
  NEIII               1.00      55747.000
  NEIII               5.00     204292.000
  NEIII               3.00     204879.000
  NEIII               1.00     205204.000
  NEIII               3.00     289479.000
  NEIII               5.00     314148.000
  NEIII               3.00     319444.875
  NEIII              15.00     352745.875
  NEIII              15.00     353148.000
  NEIII               9.00     356776.500
  NEIII               5.00     357930.000
  NEIII               9.00     374434.000
  NEIII               3.00     379834.000
  NEIII               8.00     389069.312
  NEIII               7.00     389139.000
  NEIII              21.00     391450.250
  NEIII              45.00     398946.937
  NEIII               4.00     399082.562
  NEIII              15.00     409847.500
  NEIII              12.00     412320.187
  NEIII              75.00     436561.312
56          NE+++   0 0 0 0 0 1 0-3 0 0 20.18135 01  29 0.0
NE+++  HEAT FORM      .291405E 04
  NEIV                4.00          0.0
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  NEIV                10.00     40950.000
  NEIV                 6.00     62167.000
  NEIV                 6.00    183860.000
  NEIV                 4.00    184477.000
  NEIV                 2.00    184799.000
  NEIV                10.00    253807.000
  NEIV                 2.00    299351.000
  NEIV                 6.00    319751.000
  NEIV                12.00    479651.000
  NEIV                 6.00    484623.000
  NEIV                 6.00    488917.000
  NEIV                10.00    511411.000
  NEIV                16.00    525017.000
  NEIV                 2.00    551712.000
  NEIV                34.00    579375.000
  NEIV                22.00    580095.000
  NEIV                24.00    605417.000
  NEIV                 8.00    612781.000
  NEIV                18.00    634413.000
  NEIV                36.00    642934.000
  NEIV                10.00    664124.000
  NEIV                56.00    672799.000
  NEIV                36.00    697855.000
  NEIV                 0.0     697855.000
  NEIV                16.00    709460.000
  NEIV                10.00    724690.000
  NEIV                14.00    740607.000
  NEIV                10.00    754597.000
57          HE+     0 0 0 0 0 0 1-1 0 0  4.00205 01    5 0.0
 HE+ HEAT FORMATION  .566930E+03
  HEII                2.00         0.0
  HEII                8.00    329184.937
  HEII               18.00    390142.875
  HEII               32.00    411478.000
  HEII               50.00    421353.062
58          HE++    0 0 0 0 0 0 1-2 0 0  4.00150 05    0 0.0
 HE++HEAT FORMATION  .182102E+04
59           C      1 0 0 0 0 0 0 0 0 0 12.01115 01   4I 0.0
 C   HEAT FORMATION 0.169990E 03
   CI                1.00         0.0
   CI                3.00        16.400
   CI                5.00        43.500
   CI                5.00     10193.699
   CI                1.00     21648.398
   CI                5.00     33735.199
   CI                4.00     60353.000
   CI                8.00     60393.520
   CI               15.00     64088.559
   CI                3.00     68858.000
   CI               15.00     69744.375
   CI                3.00     70744.250
   CI                9.00     71385.687
   CI                5.00     72611.000
   CI                1.00     73976.187
   CI                9.00     75256.250
   CI                5.00     77680.500
   CI               14.00     78199.312
   CI               31.00     78250.187
   CI                3.00     78338.000
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   CI                  7.00     78531.000
   CI                  3.00     78727.875
   CI                  9.00     79311.062
   CI                 18.00     80222.687
   CI                 12.00     81344.437
   CI                  6.00     81770.312
   CI                 51.00     83761.000
   CI                 30.00     84986.187
   CI                 11.00     86187.000
   CI                 46.00     86326.875
   CI                 12.00     86504.000
   CI                 26.00     87713.000
   CI                 37.00     87807.000
   CI                 21.00     88547.000
   CI                 34.00     88624.000
   CI                 21.00     89081.000
   CI                 31.00     89155.000
   CI                 21.00     89450.000
   CI                 22.00     89517.000
   CI                 15.00     89779.000
   CI                 15.00     89968.375
60          N      0 1 0 0 0 0 0 0 0 0 14.0067  01  51 0.0
 N   HEAT FORMATION 0.112507E 03
  NI                  4.00         0.0
  NI                 10.00     19223.000
  NI                  6.00     28840.000
  NI                 12.00     83366.000
  NI                  6.00     86223.187
  NI                 12.00     88109.500
  NI                  2.00     93582.250
  NI                 20.00     94883.062
  NI                 12.00     95533.187
  NI                 14.00     96864.187
  NI                  6.00     97805.750
  NI                 10.00     99665.000
  NI                 12.00    103736.750
  NI                  6.00    104227.375
  NI                 34.00    104767.000
  NI                 32.00    104882.687
  NI                 24.00    105020.000
  NI                  2.00    106478.562
  NI                  6.00    106780.062
  NI                 20.00    106870.687
  NI                 10.00    107039.000
  NI                 12.00    109927.875
  NI                  2.00    110029.187
  NI                  8.00    110196.000
  NI                 32.00    110248.000
  NI                 38.00    110304.000
  NI                 16.00    110470.500
  NI                 10.00    110545.750
  NI                  6.00    112320.750
  NI                  2.00    112565.875
  NI                 10.00    112682.562
  NI                 20.00    112799.000
  NI                 60.00    112862.000
  NI                 16.00    112947.500
  NI                  6.00    114072.000
  NI                 62.00    114160.000
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  NI                  40.00    114275.000
  NI                   6.00    114890.000
  NI                  32.00    114988.000
  NI                  24.00    115004.000
  NI                  18.00    115103.000
  NI                  18.00    115483.000
  NI                  44.00    115535.000
  NI                  18.00    115618.000
  NI                  44.00    115887.000
  NI                  36.00    115902.000
  NI                  58.00    116164.000
  NI                  22.00    116259.000
  NI                  58.00    116367.000
  NI                  28.00    116441.000
  NI                  28.00    116625.000
61          O       0 0 1 0 0 0 0 0 0 0 0 15.99940 01   32 0.0
 O   HEAT FORMATION 0.589725E 02
  O                   5.00         0.0
  O                   3.00       158.500
  O                   1.00       226.500
  O                   5.00     15867.699
  O                   1.00     33792.398
  O                   5.00     73767.750
  O                   3.00     76794.687
  O                  15.00     86631.000
  O                   9.00     88630.812
  O                   5.00     95476.375
  O                   3.00     96225.500
  O                  45.00     97420.187
  O                  15.00     99094.500
  O                   9.00     99680.375
  O                  15.00    101135.000
  O                   5.00    102116.187
  O                   3.00    102411.625
  O                   5.00    102661.625
  O                  25.00    102865.062
  O                  15.00    102908.125
  O                   9.00    103869.375
  O                   8.00    105019.000
  O                  40.00    105385.250
  O                   9.00    105911.250
  O                   8.00    106545.062
  O                  40.00    106751.187
  O                   8.00    107445.375
  O                  40.00    107573.062
  O                   8.00    108021.375
  O                  40.00    108105.687
  O                  48.00    108470.187
  O                  48.00    108731.500
62          H       0 0 0 1 0 0 0 0 0 0 0  1.00797 01    6 0.0
 H   HEAT FORMATION  .516200E+02
  H                   2.00         0.0
  H                   8.00     82259.250
  H                  18.00     97492.312
  H                  32.00    102823.875
  H                  50.00    105291.625
  H                  72.00    106632.125
63          AR      0 0 0 0 1 0 0 0 0 0 39.94800 01   59 0.0
 A HEAT FORMATION   0.         E 00
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AI	1.00	0.0
AI	5.00	93143.750
AI	3.00	93750.625
AI	1.00	94553.687
AI	3.00	95399.812
AI	3.00	104102.125
AI	12.00	105462.750
AI	8.00	106237.562
AI	13.00	107289.687
AI	4.00	111818.062
AI	21.00	112750.187
AI	20.00	113716.562
AI	8.00	114641.000
AI	19.00	114821.937
AI	15.00	116942.812
AI	8.00	117183.625
AI	1.00	117563.000
AI	15.00	118469.062
AI	22.00	119023.687
AI	5.00	119444.875
AI	12.00	119566.062
AI	6.00	119847.750
AI	8.00	120188.625
AI	48.00	120207.312
AI	10.00	120619.062
AI	7.00	120753.500
AI	7.00	121068.750
AI	23.00	121165.375
AI	30.00	121653.375
AI	17.00	122036.125
AI	12.00	122160.187
AI	12.00	122329.687
AI	6.00	122514.250
AI	68.00	122695.687
AI	23.00	123205.812
AI	9.00	123372.937
AI	13.00	123557.437
AI	16.00	123653.187
AI	35.00	123832.500
AI	84.00	124046.625
AI	23.00	124349.000
AI	5.00	124554.937
AI	37.00	124609.875
AI	75.00	124860.625
AI	28.00	125054.062
AI	17.00	125150.000
AI	39.00	125219.875
AI	68.00	125388.625
AI	53.00	125482.687
AI	36.00	125631.687
AI	78.00	125750.375
AI	61.00	125922.500
AI	76.00	126135.375
AI	80.00	126295.750
AI	84.00	126517.375
AI	12.00	127130.000
AI	12.00	127410.000
AI	24.00	127760.000
AI	16.00	127970.000

```
64          NE     0 0 0 0 0 1 0 0 0 0 20.18300 01  25 0.0
 NE  HEAT FORMATION  .000000E+00
  NE                   1.00         0.0
  NE                   5.00    134043.750
  NE                   3.00    134461.187
  NE                   1.00    134820.562
  NE                   3.00    135890.625
  NE                   3.00    148259.687
  NE                  12.00    149659.000
  NE                   8.00    150317.812
  NE                   9.00    150860.437
  NE                   3.00    151040.375
  NE                   1.00    152972.687
  NE                   8.00    158603.062
  NE                   4.00    159536.562
  NE                  40.00    161592.250
  NE                  35.00    162832.625
  NE                  20.00    163710.562
  NE                   9.00    165830.125
  NE                   8.00    166977.312
  NE                 148.00    167062.500
  NE                  20.00    168926.625
  NE                 124.00    169536.250
  NE                 148.00    170879.937
  NE                 216.00    171689.937
  NE                 428.00    172575.812
  NE                 188.00    173280.000
65          HE     0 0 0 0 0 0 1 0 0 0  4.00260001  16 0.0
HE   HEAT FORMATION  .000000E 00
  HE                   1.00         0.0
  HE                   3.00    159850.312
  HE                   1.00    166271.687
  HE                  12.00    169081.062
  HE                   3.00    183231.062
  HE                   1.00    184859.000
  HE                   9.00    185558.875
  HE                  23.00    186095.875
  HE                   4.00    190292.437
  HE                  60.00    191446.562
  HE                  13.00    193795.062
  HE                  51.00    193915.750
  HE                  68.00    195256.812
  HE                 188.00    196950.312
  HE                 340.00    197398.562
  HE                  78.00    198056.500
66          E-     0 0 0 0 0 0 0 1 0 0  0.00054905   0 0.0
 E-  HEAT FORMATION 0.       E 00
```

Nomenclature

B_i concentration of the ith element at STP, moles/l.

C_i quantity defined in Eq. (46).

D_i constant defined with Eqs. (44) and (45).

f_i^o partial molal free energy of the ith specie evaluated at a pressure of one atmosphere, cal/mole.

$g_i^{(k)}$ degeneracy of the ith energy level of the kth specie.

H enthalpy per unit mass.

h_i^o partial molal enthalpy of the ith specie evaluated at a pressure of one atmosphere, cal/mole.

h_{oi}^o energy of formation for one mole of the ith specie at a pressure of one atmosphere and a temperature of 0°K, cal/mole.

K thermal conductivity.

M_o molecular weight at standard conditions (cold molecular weight).

$N_i^{(k)}$ number of particles of the kth constituent.

n_i concentration of the ith specie, mole/l.

$N_i^{(k)}$ number of particles of the kth constituent in the ith energy level.

P total pressure of mixture.

P_i partial pressure of the ith specie.

R universal gas constant, 1.98726 cal/mole – °K.

S entropy per unit mass.

T temperature, °K.

U velocity.

v $= 1/\rho$ specific volume of gas, l/g

$X^{(j)}$ the chemical symbol for the jth numbered chemical element.

$Y^{(i)}$ the chemical symbol for the ith numbered compound.

Y_{ij} matrix coefficient defined in Eq. (46).

Z $= \dfrac{M_o}{M}$

α_{ij} the number of atoms of the jth numbered element in the molecule of the *ith* numbered specie.

$\epsilon_i^{(k)}$ energy of the ith level for the kth specie.

η viscosity.

ρ mass density.

ρ_o density of mixture at STP.

$(\ )_o$ property of mixture at STP.

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