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TECHNICAL NOTE

D-1454

A GENERAL IBM 704 OR 7090 COMPUTER PROGRAM FOR COMPUTATION OF CHEMICAL EQUILIBRIUM COMPOSITIONS, ROCKET PERFORMANCE, AND CHAPMAN-JOUGUET DETONATIONS

By Frank J. Zeleznik and Sanford Gordon

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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ERRATA

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FOR COMPUTATION OF CHEMICAL EQUILIBRIUM

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Page 17: Equation (47) should read

$$\mathscr{F}_c - \mathscr{F}_g \leq 0$$

Page 25, line 15: Immediately following the sentence ending with the word "constant" insert the following sentences:

It should be noted that the four functions described above do not destroy the contents of the multiplier-quotient register, C(MQ), although C(MQ) may be altered as a result of the shifting. This fact is used in some portions of the program to avoid storing C(MQ). Therefore any routines written to replace the functions discussed here must not destroy C(MQ).

Page 25, line 23: Immediately preceding the last paragraph insert the following paragraphs:

In addition to the program input to be discussed in the section PROGRAM INPUT DATA, thermodynamic data must be supplied to the program. These data are assumed to be available as a master data tape, which must be loaded onto tape handler number four at the start of computation and unloaded when the computations have been completed. Since this master data tape is used for both reading and writing it cannot be file protected. Loading and unloading the data tape is time consuming and costly. It has been found to be economical to make the data tape from binary cards rather than to stop the computer for loading and unloading the data tape. The following changes will permit operation in this fashion. For the IBM 7090 program, replace card number 123, page 87 (PAUSE 11111) with

```
5000   REWIND 4
       CALL BCREAD (DATA(44), DATA(1))
       DATA(23)=DATA(26)
       WRITE TAPE 4, (DATA(I), I=1, 23)
       IF (MDATA(1)-MEND) 5000, 429, 5000
```

Also remove card number 332, page 88 (PAUSE 77777). The corresponding change for the IBM 704 program involves replacing card number 106, page 50, (PAUSE 11111) with

```
5000    REWIND 4
        CALL BCREAD (DATA(44), DATA(1))
        DATA(23)=DATA(26)
        WRITE TAPE 4, (DATA(I), I=1, 23)
S       CLA DATA(1)
S       SUB END
S       TNZ*5000
```

and removing card number 432, page 53 (PAUSE 77777). If these changes are made, then the master data tape is no longer needed but the equivalent binary cards must be available. These can be made from the master data tape.

These changes use the Subroutine BCREAD (A,B). This subroutine is part of a computer system at the Lewis Research Center and is not given in this report; however, its only function is to read binary cards punched by a companion Subroutine BCDUMP (A,B). In both cases the arguments A and B are, respectively, the first and last words to be read or punched. Each binary card contains 22 words of information and thus, since the data for each species requires 23 words (see fig. 6), two cards are required for each species. The first of each pair of cards contains the first 22 words while the second card of each pair contains the 23rd word plus the first 3 words of the record for identification purposes. These two subroutines are not essential and can be replaced by any equivalent subroutines or sequence of instructions.

Page 62: Replace card number 1418, statement number 1126, with

```
        IF (EN LN(J)) 2125, 1126, 2125
2125    P=P+EXPF(EN LN(J))
1126    CONTINUE
```

Page 64: Replace card number 1709, statement number 309, with

```
309     PCP(25)=PCP(IADD)
        IADD=25
```

Page 96: Replace card number 1033, statement number 1031, with

```
1031    IF (WF) 1050, 1050, 1040
```

Page 96: Replace card number 1039 with

```
1050    DO 2000 I=1,15
```

Page 99: Replace card number 1333 with

```
        IF (ABSF(D LN T)-ABSF(X(IQ1))) 501, 913, 913
```

Page 99: Replace card number 1341 with

```
        IF (DEL N(J)) 917, 917, 1917
```

Page 99: Replace card number 1374, statement number 1126, with

```
      IF (EN LN(J)) 2125, 1126, 2125
2125  P=P+EXPF(EN LN(J))
1126  CONTINUE
```

Page 102: Replace card number 1656, statement number 309, with

```
309   PCP(25)=PCP(IADD)
      IADD=25
```

NASA-Langley, 1963

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

TECHNICAL NOTE D-1454

A GENERAL IBM 704 OR 7090 COMPUTER PROGRAM FOR COMPUTATION OF CHEMICAL EQUILIBRIUM COMPOSITIONS, ROCKET PERFORMANCE, AND CHAPMAN-JOUGUET DETONATIONS

By Frank J. Zeleznik and Sanford Gordon

SUMMARY

A detailed description of a computer program for computations involving chemical equilibrium in complex systems is given. It is based on iteration equations for chemical equilibrium computations that are independent of choice of components. The program permits calculations such as: (1) chemical equilibrium for assigned temperatures and pressures, (2) theoretical rocket performance for both frozen and equilibrium compositions during expansion, and (3) Chapman-Jouguet detonation properties.

A discussion of some of the problems attendant with the presence of condensed species as reaction products is also given.

INTRODUCTION

The problem of the numerical solution of the nonlinear algebraic equations describing chemical equilibrium has been the subject of numerous papers. Reference 1 contains an extensive bibliography on the subject prior to 1959. Since the publication of reference 1, many additional papers have been written dealing with the computation of chemical equilibrium properties (refs. 2 to 16). Some of the references describe programs for digital computers. Reference 1, for example, contains a detailed description of a program written at the Lewis Research Center for the IBM 650 to calculate equilibrium compositions and rocket performance.

The purpose of this report is to describe in detail a computer program written at the Lewis Research Center for the IBM 704 and 7090 for the computation of chemical equilibrium in complex systems with several applications. Use has been made of the modified Huff method described in reference 15, which permits iteration equations to be written in a form independent of the choice of components. The program can perform the following calculations: (1) chemical equilibrium for assigned temperatures and pressures, (2) theoretical rocket performance for both frozen and equilibrium composition during expansion, and (3) Chapman-Jouguet detonation properties.

The objective has been to develop a program that can compute equilibrium compositions for any chemical system for which thermodynamic data exist. To accomplish this objective, several special techniques were incorporated to handle problems that would otherwise not converge. These techniques, which have proven successful in the many problems attempted, include a flexible convergence control parameter, automatic inclusion of condensed species with the possibility of triple points, and a pivoting procedure during solution of the iteration equations.

The computer program will be described in the following sections of the report with sufficient detail to permit its use. The following are some of its general features:

(1) It requires only simple input.

(2) It requires no initial estimates.

(3) It handles up to 15 chemical elements and a total of 90 reaction products including condensed species.

SUMMARY OF EQUATIONS USED IN THE PROGRAM

The derivations of equations used in the program and a discussion of the assumptions involved have been previously published (refs. 1, 15, 17, 18, and 19). However, for convenience in describing the computer program, the pertinent equations from these references will be summarized in this report.

The notation of these references was used when possible. However, since the notation in all these references is not exactly the same, complete consistency was not possible, in particular for thermodynamic functions. In this report, for heat capacity, enthalpy, entropy, and free energy, a capital Roman letter refers to the quantity per mole, while a capital script letter is the dimensionless form (which, in the case of entropy and free energy, may include additional dimensionless terms). A lower-case Roman letter is the quantity per unit mass, while a lower-case script letter has the units of moles per unit mass of reactant.

Equilibrium Compositions and Properties of Complex Mixtures

The equilibrium compositions are obtained by a Newton-Raphson iteration. The iteration equations are those of the modified Huff method, which were derived in reference 15 and are presented in figure 2 of that report. These equations are presented herein as table I with symbols altered to correspond to those used in this report. The corrections to the estimates that are obtained from this set of iteration equations are unaffected by the choice of components and are only affected by the current estimates. These equations make no distinction between components and constituents, and thus any species can be dropped from the calculation. The iteration equations give corrections to the moles of each condensed species and the variables A and T directly. (Symbols are defined in appendix A.) The corrections to the moles of gaseous species are obtained from the following equation (see eq. (88), ref. 15):

$$\Delta \ln n_i = -\mathscr{F}_i + \sum_{k=1}^{l} a_{ki} \Delta \ln u_k + \mathscr{H}_i \Delta \ln T \qquad (i = 1, 2, \ldots, m) \tag{1a}$$

It is sometimes disadvantageous to apply the entire correction called for by the iteration equations. Consequently an empirical convergence parameter $\lambda (0 < \lambda \leq 1)$ is used to control the size of the corrections. A numerical value for λ is determined at each iteration. Methods for evaluating λ are discussed in the section Evaluation of Convergence Parameter λ. New estimates are obtained from the following equations:

$$\left.\begin{aligned}
\ln n_i^{(j+1)} &= \ln n_i^{(j)} + \lambda \Delta \ln n_i \qquad (i = 1, 2, \ldots, m)\\
n_i^{(j+1)} &= n_i^{(j)} + \lambda \Delta n_i \qquad (i = m+1, m+2, \ldots, n)\\
\ln A^{(j+1)} &= \ln A^{(j)} + \lambda \Delta \ln A\\
\ln T^{(j+1)} &= \ln T^{(j)} + \lambda \Delta \ln T
\end{aligned}\right\} \tag{1b}$$

The indices j and j+1 signify the estimates for the j^{th} and $(j+1)^{st}$ iterations. When the iteration has converged, the moles of gaseous species n_i will be numerically equal to the partial pressures $p_i (i = 1, 2, \ldots, m)$.

After the equilibrium compositions have been determined, the three independent first derivatives c_p, $(\partial \ln M/\partial \ln T)_P$, and $(\partial \ln M/\partial \ln P)_T$ can be evaluated by a procedure analogous to that described in reference 1. The calculation of c_p and $(\partial \ln M/\partial \ln T)_P$ requires the derivatives $(\partial \ln n_i/\partial \ln T)_P$ $(i = 1, 2, \ldots, m)$, $(\partial n_i/\partial \ln T)_P$ $(i = m + 1, m + 2, \ldots, n)$, and $(\partial \ln A/\partial \ln T)_P$. Following the procedure of reference 15 for the elimination of linear combination terms, the set of equations in table II is obtained for the derivatives $(\partial \ln u_i/\partial \ln T)_P$ $(i = 1, 2, \ldots, l)$, $(\partial n_i/\partial \ln T)_P$ $(i = m + 1, m + 2, \ldots, n)$, and $(\partial \ln A/\partial \ln T)_P$. The $(\partial \ln n_i/\partial \ln T)_P$ are related to these by

$$\left(\frac{\partial \ln n_i}{\partial \ln T}\right)_P = \sum_{k=1}^{l} a_{ki}\left(\frac{\partial \ln u_k}{\partial \ln T}\right)_P + \mathcal{H}_i \qquad (i = 1, 2, \ldots, m) \tag{2a}$$

Writing the equation for evaluating the specific heat (eq. (42), ref. 1) in the notation of this report and substituting equation (2a) in it give

$$c_p = \frac{R}{A}\left[\sum_{k=1}^{l}\sum_{i=1}^{m} a_{ki}\mathcal{H}_i n_i\left(\frac{\partial \ln u_k}{\partial \ln T}\right)_P + \sum_{i=m+1}^{n} \mathcal{H}_i\left(\frac{\partial n_i}{\partial \ln T}\right)_P + \sum_{i=1}^{m} \mathcal{H}_i n_i\left(\frac{-\partial \ln A}{\partial \ln T}\right)_P + \sum_{i=1}^{m} \mathcal{C}_i n_i + \sum_{i=1}^{m} \mathcal{H}_i\mathcal{H}_i n_i\right] \tag{2b}$$

The solution of the equations in table II also gives one of the molecular weight derivatives by means of the relation

$$\left(\frac{\partial \ln M}{\partial \ln T}\right)_P = \left(\frac{\partial \ln A}{\partial \ln T}\right)_P \tag{3a}$$

The derivative $(\partial \ln M/\partial \ln P)_T$ can be calculated from

$$\left(\frac{\partial \ln M}{\partial \ln P}\right)_T = \frac{P}{\sum_{k=1}^{l}\sum_{i=1}^{m}\left(a_{ki}n_i \frac{\partial \ln u_k}{\partial \ln A}\right)_T} - 1 \tag{3b}$$

where the required partial derivatives in (3b) are obtained by a solution of the equations of table III of this report. The equations (3a) and (3b) and the equations of table III are identical, respectively, to equations (48) and (51) and figure 4 of reference 1 except for notation. It should be noted that the matrix elements of tables II and III are identical with the corresponding elements of table I except for the sign of the last column in table II. The isentropic exponent γ used in the calculations of the velocity of sound is

$$\gamma \equiv \left(\frac{\partial \ln P}{\partial \ln \rho}\right)_s = \frac{1}{\left[1 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] - \frac{R}{c_p M}\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]^2} \tag{4}$$

Frozen Composition and Properties of Complex Mixtures

In addition to the properties of a complex mixture under conditions of chemical equilibrium, it is sometimes desirable to obtain properties of the mixture for a fixed composition. The technique for doing this has been discussed in reference 1. The procedure employed here is identical except it has been found convenient to use the composition in terms of mole fractions. For a mixture of fixed composition, entropy, and pressure, the temperature is calculated by a Newton-Raphson iteration. The correction to the current estimate for temperature is obtained from

$$\Delta \ln T = \frac{\mathcal{S}_f - \mathcal{S}_f^o}{\sum_{i=1}^{n} \mathcal{C}_i x_i} \tag{5a}$$

The improved estimate for temperature is then obtained by means of

$$\ln T^{(j+1)} = \ln T^{(j)} - \Delta \ln T \tag{5b}$$

For frozen composition, the three independent first partial derivatives are:

$$c_p = R \frac{\sum_{i=1}^{n} \mathscr{C}_i x_i}{M_c \sum_{i=1}^{m} x_i} \tag{6}$$

and

$$\left(\frac{\partial \ln M}{\partial \ln T}\right)_P = 0 \tag{7}$$

and

$$\left(\frac{\partial \ln M}{\partial \ln P}\right)_T = 0 \tag{8}$$

The isentropic exponent γ is

$$\gamma = \frac{c_p M_c}{c_p M_c - R} \tag{9}$$

Rocket Performance Parameters

The evaluation of rocket performance parameters for a propellant is simple once the temperature and composition are known at combustion and exit points of a nozzle. The temperature and composition in the combustion chamber and at all exit points, with the exception of the throat, can be determined by the previous iteration equations. The throat conditions are evaluated with the aid of a secondary Newton-Raphson iteration using the equation

$$\left(\frac{P_c}{P}\right)_{k+1} = \frac{\left(\frac{P_c}{P}\right)_k}{1 + \frac{2M\left(h_c - h_k^*\right)}{(\gamma + 1)RT}} \tag{10}$$

where $(P_c/P)_k$ is the k^{th} estimate for pressure ratio at the throat and h_k^* is the value of h^* for the pressure corresponding to this pressure ratio and an entropy equal to the combustion entropy. This procedure is identical to the one described in reference 1. The method used to obtain the initial estimate for P_c/P and T at the throat is described in a later section.

The following formulas used in computing the various performance parameters were derived from the one-dimensional forms of continuity, energy, and momentum equations and the following assumptions: zero velocity in the combustion chamber, perfect gas law, complete combustion, homogeneous mixing, adiabatic combustion, and isentropic expansion. (The units used were h = cal/g, T = °K, P = lb force/sq in., A = sq in., w = lb mass/sec, and g_c = 32.174 (lb mass/lb force)(ft/sec^2).)

Specific impulse with ambient and exit pressures equal, (lb force)(sec)/lb mass:

$$I = 294.98 \sqrt{\frac{h_c - h}{1000}} \tag{11}$$

Specific impulse in vacuum (ambient pressure zero), (lb force)(sec)/lb mass:

$$I_{vac} = I + P \frac{A}{w} \tag{12}$$

Nozzle area per unit mass-flow rate, (sq in.)(sec)/lb:

$$\frac{A}{w} = \frac{86.4579\ T}{PMI} \tag{13}$$

Characteristic velocity, ft/sec:

$$c^* = g_c P_c \left(\frac{A}{w}\right)_t = 32.174\ P_c \left(\frac{A}{w}\right)_t \tag{14}$$

Coefficient of thrust:

$$C_F = \frac{g_c I}{c^*} = 32.174\ \frac{I}{c^*} \tag{15}$$

Mach number:

$$\mathscr{M} = \frac{U}{U_s} = \frac{I}{\sqrt{\frac{86.4579\ \gamma T}{M}}} \tag{16}$$

The derivatives of these performance parameters and their use for extrapolation and interpolation of rocket performance calculation are discussed in reference 17. The formulas for calculating these derivatives are given in table IV. The program calculates the derivatives of

T, I, ϵ, and c^* only. The remaining derivatives can be calculated from these and other equilibrium properties using the equations in table IV.

Chapman-Jouguet Detonations

The thermodynamic calculation of the properties of a Chapman-Jouguet detonation are discussed in reference 18. The calculation involves a Newton-Raphson iteration to determine detonation conditions in addition to the previously described iteration for determining equilibrium compositions. The detonation iteration equations are presented here as table V. Reference 18 also presents a method for evaluating the partial derivatives of the detonation velocity, pressure ratio, and temperature ratio and discusses their use in extrapolating detonation data. The equations for evaluating the required partial derivatives are presented here as table VI. When detonation conditions have been determined, the detonation velocity in meters per second can be calculated as

$$U_D = 91.1845 \frac{\rho}{\rho_1} \sqrt{\frac{\gamma T}{M}} \tag{17}$$

where T is in $^{\circ}K$.

Thermodynamic Data

The thermodynamic data used by the program must be in the form of empirical equations; thus

$$\frac{C_p^{\circ}}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \tag{18}$$

and

$$\frac{H_T^{\circ}}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \tag{19}$$

and

$$\frac{S_T^{\circ}}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} T^3 + \frac{a_5}{4} T^4 + a_7 \tag{20}$$

The constants $a_i (i = 1, 2, \ldots, 7)$ can be evaluated by the least-squares method of reference 19 for one or more temperature intervals.

Continuity of the three functions across intervals is assured by the aforementioned method since it requires that the residuals vanish at the first point of each interval. The equations for determining the constants are given in table VII. Appendix B lists coefficients for 224 substances obtained by means of the equations in table VII. The coefficients for most substances cover the range from 300° to 5000° K in the two intervals 300° to 1000° K and 1000° to 5000° K.

The enthalpy base selected was an assigned value of zero at 298.15° K for the reference substances: Al(s), Be(s), C(graphite), Cl_2(g), F_2(g), H_2(g), Li(s), Mg(s), N_2(g), Na(s), O_2(g), P(white), S(rhombic), and Si(c), and zero at 0° K for Ar(g), He(g), and Ne(g).

The value $H^O_{298.15}$ for a substance formed from any of these reference substances except the inert gases is its heat of formation relative to these substances at 298.15° K. For example, for CO_2, $H_{298.15} = \Delta H_{298.15} = -94{,}051.8$ cal/mole, which can be obtained from the coefficients in the 300° to 1000° K interval with $T = 298.15^\circ$ K.

Input Calculations

The input calculations are identical to those described in reference 1. For convenience they will be described in this report. The reactants are divided into two groups, fuels and oxidants. The fuels are those reactants which will be primarily oxidized, while oxidants are those reactants which will be primarily reduced. The fuels can be combined into an effective fuel by specifying the relative proportions of each fuel. Similarly, the oxidants can be combined into an effective oxidant by specifying the relative proportions of the oxidants. The overall composition (i.e., the b_i^O's) can be calculated by specifying the relative amounts of the effective oxidant and effective fuel. This method of assigning the overall composition is particularly convenient if calculations are to be performed for various relative amounts of effective oxidant and effective fuel. The gram-atoms of the i^{th} element per gram of effective oxidant or of effective fuel are, respectively,

$$\left(b_x^o\right)_i = \frac{1}{\sum_k W_k^x} \sum_j a_{ij}^x \frac{W_j^x}{M_j^x} \qquad (21a)$$

or

$$\left(b_f^o\right)_i = \frac{1}{\sum_k W_k^f} \sum_j a_{ij}^f \frac{W_j^f}{M_j^f} \tag{21b}$$

In terms of these equations, the gram-atoms per gram of reactant b_i^o can be calculated as

$$b_i^o = \frac{\left(b_f^o\right)_i + (O/F)\left(b_x^o\right)_i}{1 + (O/F)} \tag{22}$$

Formulas analogous to formulas (21) and (22) are used to calculate the following enthalpies:

Enthalpy per gram of effective oxidant:

$$h_x = \frac{1}{\sum_k W_k^x} \sum_j \left(H_T^o\right)_j^x \frac{W_j^x}{M_j^x} \tag{23a}$$

Enthalpy per gram of effective fuel:

$$h_f = \frac{1}{\sum_k W_k^f} \sum_j \left(H_T^o\right)_j^f \frac{W_j^f}{M_j^f} \tag{23b}$$

Enthalpy per gram of reactant:

$$h_0 = \frac{h_f + (O/F)h_x}{1 + (O/F)} \tag{24}$$

The relative amounts of effective oxidant and fuel are sometimes given as the weight percent of fuel $\%F$, which is related to the oxidant-to-fuel weight ratio O/F by

$$\%F = \frac{100}{1 + (O/F)} \tag{25}$$

A third way of specifying the relative amounts of oxidant and fuel is by means of an equivalence ratio, which can be related to O/F. Let V_i^+ and V_i^- be the positive and negative oxidation states of an element in its commonly occurring compounds. At least one of these will be zero. Thus, for example, the negative oxidation state for chlorine is -1 and its positive oxidation state is zero. In terms of the common oxidation states for the elements, oxidation states per gram of effective oxidant and fuel are

$$V_x^+ = \sum_{j=1}^{l} V_j^+ \left(b_x^o\right)_j \tag{26}$$

$$V_x^- = \sum_{j=1}^{l} V_j^- \left(b_x^o\right)_j \tag{27}$$

$$V_f^+ = \sum_{j=1}^{l} V_j^+ \left(b_f^o\right)_j \tag{28}$$

$$V_f^- = \sum_{j=1}^{l} V_j^- \left(b_f^o\right)_j \tag{29}$$

where the sum is over the various elements. In terms of these four quantities, the positive and negative oxidation states of the propellant are

$$V^+ = \frac{V_f^+ + (O/F)V_x^+}{1 + (O/F)} \tag{30}$$

$$V^- = \frac{V_f^- + (O/F)V_x^-}{1 + (O/F)} \tag{31}$$

The equivalence ratio is now defined as

$$\mathcal{R} \equiv -\frac{V^+}{V^-} = \frac{-V_f^+ - (O/F)V_x^+}{V_f^- + (O/F)V_x^-} \tag{32}$$

With this definition, $\mathcal{R} = 1$, $\mathcal{R} < 1$, and $\mathcal{R} > 1$ correspond to the stoichiometric, the oxidant-rich, and the fuel-rich conditions, respectively. The equivalence ratio used in this report is the reciprocal of the one used in reference 1.

INITIAL ESTIMATES

All of the iteration equations listed in the previous section require an initial set of estimates. The methods for obtaining estimates for each of the iterations will be described below.

Equilibrium Compositions

Experience has shown that for the determination of equilibrium compositions it is unnecessary to begin the iteration with a good set of estimates, although a good set of estimates will reduce the number of iterations required to converge to a solution. However, in the case of complex systems, it is often extremely difficult and time consuming to obtain a good set of composition estimates manually. The cost of a few extra iterations on the computer will be small relative to the cost of obtaining estimates manually and inserting them as part of the input information. Furthermore, in the case of rocket performance calculations, estimates are potentially useful only for combustion conditions. The results of combustion conditions serve as estimates for exit conditions. Therefore, the importance of initial estimates decreases as the number of exit points increases. Because of these considerations, the computer program to be described in later portions of this report will not accept estimates for any variable other than combustion temperature.

For the first point, the computer program uses a partial pressure of 1 atmosphere for all gaseous species and zero moles for all condensed species as initial composition estimates. If the calculation is for an assigned enthalpy and no combustion temperature estimate is given, then an estimate for temperature of about 3800° K is used. For the mass variable A, an estimate of approximately 150 grams is used. For succeeding points, the results of the preceding point are used as estimates.

Rocket Nozzle Throat

Good estimates, primarily, for throat pressure and, secondarily, for throat temperature, can result in an appreciable decrease in the number of iterations because of the presence of a secondary iteration in the calculation of throat conditions in a rocket nozzle. An excellent estimate of the throat pressure ratio for both equilibrium and frozen compositions is

$$P_c/P = \left(\frac{\gamma_c + 1}{2}\right)^{\frac{\gamma_c}{\gamma_c - 1}} \tag{33}$$

This relation usually gives a throat pressure ratio, which is correct to three places. The throat temperature is estimated from the equation

$$T = \frac{2}{1 + \gamma_c} T_c \tag{34}$$

Chapman-Jouguet Detonations

Because the Chapman-Jouguet calculation is a Newton-Raphson iteration within the Newton-Raphson iterations to determine equilibrium gas properties, it is very desirable to have good estimates for the pressure ratio and the temperature ratio across the detonation wave. A method (ref. 18) for obtaining excellent estimates of the temperature and pressure ratio will be described here briefly. Let the initial estimate for pressure ratio be $(P/P_1)_0$ and the initial estimate for temperature ratio be $(T/T_1)_0$ where T in this initial estimate is the flame temperature corresponding to an enthalpy

$$h = h_1 + \frac{3}{4} \frac{RT_1}{M_1}\left(\frac{P}{P_1}\right)_0 \tag{35}$$

The initial estimates $(P/P_1)_0$ and $(T/T_1)_0$ can be further improved by successive use of the following equations (ref. 18):

$$\left(\frac{P}{P_1}\right)_{k+1} = \frac{1 + \gamma}{2\gamma\alpha_k}\left[1 + \sqrt{1 - \frac{4\gamma\alpha_k}{(1 + \gamma)^2}}\right] \tag{36}$$

$$\left(\frac{T}{T_1}\right)_{k+1} = \left[\left(\frac{T}{T_1}\right)_0 - \frac{3}{4}\frac{R}{M_1 c_p}\left(\frac{P}{P_1}\right)_0\right] + \frac{\gamma}{2}\frac{R}{M_1 c_p}\frac{r_{k+1}^2 - 1}{r_{k+1}}\left(\frac{P}{P_1}\right)_{k+1} \tag{37}$$

where

$$\alpha_k = \left(\frac{T_1}{T}\right)_k \frac{M}{M_1} \tag{38a}$$

and

$$r_{k+1} = \alpha_k \left(\frac{P}{P_1}\right)_{k+1} \tag{38b}$$

The quantities M, γ, and c_p in equations (36) to (38) are the equilibrium properties for the conditions $(P/P_1)_0$ and $(T/T_1)_0$. The technique of obtaining good estimates for the iteration equations of table V by means of equations (36) and (37) is so successful that it has been found possible to arbitrarily set $(P/P_1)_0 = 15$ for all chemical systems.

If desired, it is also possible to calculate the detonation properties by using the equilibrium specific heat ratio κ in place of γ. The specific heat ratio and the isentropic exponent are related by the expression

$$\kappa = \gamma\left[1 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] \tag{39}$$

CONVERGENCE

Convergence in an iterative calculation involves two numerical problems: (1) how to assure numerical convergence, and (2) to determine at what stage the iteration should be terminated. Both of these are discussed in the following sections.

Evaluation of Convergence Parameter λ

When poor estimates are used in a Newton-Raphson iteration, the iteration equations will invariably give corrections that are too large (ref. 1). If these corrections were to be used directly, they could produce a nonconvergent iteration. This type of situation normally occurs in the early stages of a calculation. At later stages of the iteration when the problem seems to be converging satisfactorily, the iteration sometimes attempts to make large increases in the partial pressures of species that are present in trace amounts. In both of these cases it is essential to place some restriction on the size of the correction. This is accomplished by introducing a convergence parameter λ into equation (1b).

The numerical value of the convergence parameter λ is determined on the basis of two empirical rules, which experience has shown to be satisfactory. For the variables T, A, and n_j for those gaseous species for which $\ln(n_j/P_0) > -18.5$ and for which $\Delta \ln n_j > 0$, a number λ is defined as

$$\lambda_1 \equiv \frac{2}{\max(|\Delta \ln T|, |\Delta \ln A|, \Delta \ln n_j)} \qquad (j = 1, 2, \ldots, m) \qquad (40)$$

This limits the change in T and A and the increase in n_j, for those gaseous species whose gas phase mole fraction exceeds 10^{-8}, to a factor $e^2 = 7.3891$. For those gaseous species for which $\ln(n_j/P_0) \leq -18.5$ and $\Delta \ln n_j > 0$, a number λ_2 is defined as

$$\lambda_2 \equiv \min\left(\frac{\ln P_0 - 9.212 - \ln n_j}{\Delta \ln n_j}\right) \qquad (j = 1, 2, \ldots, m) \qquad (41)$$

This prevents a gaseous species with a mole fraction less than 10^{-8} from increasing its partial pressure so that its gas phase mole fraction would exceed 10^{-4}. The parameter λ to be used in equation (1b) is defined in terms of λ_1 and λ_2 as

$$\lambda \equiv \min(1, \lambda_1, \lambda_2) \qquad (42)$$

Criteria for Convergence

The criteria for convergence, which are used in the various iterative schemes in the program, will be briefly described. If, for some applications, the criteria seem too stringent, they can readily be relaxed by making the appropriate changes in the program.

Equilibrium compositions. - It is assumed that the iteration has converged to the correct composition when

$$\left.\begin{array}{ll} \dfrac{n_j}{\sum_{k=1}^{n} n_k} |\Delta \ln n_j| < 0.5\times10^{-5} & (j = 1, 2, \ldots, m) \\[2em] \dfrac{|\Delta n_j|}{\sum_{k=1}^{n} n_k} < 0.5\times10^{-5} & (j = m+1, m+2, \ldots, n) \end{array}\right\} \qquad (43)$$

This has the effect of insuring accuracy to five places in composition when it is expressed as mole fractions.

Throat conditions. - The throat conditions in a rocket nozzle are assumed to be satisfied if

$$\left| \frac{h_c - h^*}{h_c - h} \right| \leq 0.4\times10^{-4} \tag{44}$$

This condition in effect makes certain that the Mach number will satisfy the condition that

$$\mathcal{M} = 1 \pm 0.2\times10^{-4} \tag{45}$$

Chapman-Jouguet detonations. - The Chapman-Jouguet conditions are considered satisfied when

$$\left.\begin{aligned} &|\Delta \ln P/P_1| \leq 0.5\times10^{-5} \\ \text{and} \quad &|\Delta \ln T/T_1| \leq 0.5\times10^{-5} \end{aligned}\right\} \tag{46}$$

CONDENSED PHASES

Apart from some control on correction size there are essentially no numerical difficulties in determining equilibrium compositions in a gaseous system. A straightforward application of the iteration equations of table I produces rapid convergence to the correct answers. In principle there should similarly be no difficulty in applying these iteration equations to systems containing pure, insoluble condensed phases. Unfortunately, a consideration of pure condensed phases does in actuality produce some difficulties. The following sections discuss some of the problems that are encountered and present, when possible, methods for their solution. Some of these methods have been incorporated into the computer program.

Condensation

The condition for inclusion of the condensed species in the calculation can be easily derived if it is assumed that the equilibrium composition of the system without the condensed species is known at the assigned conditions and that the condensed species under consideration has a vapor form. This has been done in reference 1, and the condition is based on the fact that the condensation will occur when the partial pressure of a species is greater than or equal to the vapor pressure. From reference 1, the condition for inclusion of a condensed species in the calculation is

$$\mathscr{F}_c - \mathscr{F}_g \leq 0 \qquad (47)$$

see errata

where the subscripts c and g indicate condensed and gaseous phases, respectively.

When the condensed species does not have a corresponding vapor form, the inequality (eq. (47)) is no longer applicable. The only recourse is to include the condensed species in the iteration. If its converged value is negative, then it must be removed from the calculation and the composition redetermined. The only species of this type in appendix B is aluminum oxide (Al_2O_3). One of its condensed phases will almost certainly be present in any system containing aluminum and oxygen and, therefore, should be assumed present at the start of the iteration.

Phase Transitions and Triple Points

The calculation method is based on the assumption that condensed phases are pure. Therefore, the possibility exists of encountering phase transition between solid and liquid (melting points) or between two stable solid phases. Such transitions constitute triple points since three phases of the same species coexist, one gaseous and two condensed. Such triple points are characterized by a definite vapor pressure and temperature, independent of the relative proportions of each phase. This is shown by the fact that the iteration equations of table I become singular for an assigned temperature and pressure and the inclusion of two condensed phases of the same species. At a triple point, for a specified system pressure, the relative amounts of the phases can be determined only if either the enthalpy or the entropy is assigned.

The problem of determining equilibrium conditions in the vicinity of a phase transition can be best discussed by consideration of an example. Assume that the state is specified by an assigned pressure and an assigned entropy per unit mass, and let the phase transition be the solid-liquid transition with the transition temperature T_m (i.e., the melting temperature). An analysis for assigned enthalpy, similar to that to be given for assigned entropy, could also be made. However, in rocket performance calculations triple points occur most often at the exit points of a nozzle, and, therefore, only the assigned entropy problem will be treated in detail. Figure 1 sketches the typical dependence of system entropy upon temperature for a constant pressure. The dashed extension of the liquid-vapor curve $\overline{P_2P_5}$ would be the system entropy if the liquid were stable below the melting point. A similar statement holds for the extension of the solid-vapor curve $\overline{P_3P_6}$. At P_2 all of the condensed phase is liquid, while at P_3 all of the condensed phase is solid. Intermediate points correspond to various relative amounts of liquid and solid phases. Along the extension $\overline{P_1P_2}$ the solid phase is present in negative amounts, while along $\overline{P_3P_4}$ the amount of liquid is negative.

Two situations will be considered. First let the assigned entropy have the value s_1. If only the data for the liquid phase are used, the iteration will converge to the temperature T_l'. Since this temperature is below the melting point, the liquid phase cannot exist; therefore, the data for the liquid phase must be replaced with data for the solid phase. This time the iteration will converge to the correct temperature T_s'. Consider next the situation where the assigned entropy has the value s_2 where $s_s < s_2 < s_l$. With only the liquid phase present, the converged temperature is T_l. Since this temperature is lower than the melting point, this cannot be the correct answer. If the calculation is repeated, this time using the data for the solid phase, the calculation will converge to a temperature T_s. This again is not the correct answer since T_s is greater than the melting point. Returning to the liquid phase again produces convergence to T_l, and the calculation, if allowed to continue in this manner, would oscillate between T_l and T_s. It is apparent (fig. 1) that the correct temperature T_m can only be obtained by a simultaneous consideration of both solid and liquid phases in the iteration.

The problem of oscillatory behavior can be eliminated by specifying that in going from a consideration of liquid phase to consideration of a solid phase the intermediate situation of coexistence of solid and liquid must always be considered. This technique will always work. Take again the case where the assigned entropy is s_1. After the temperature T_l' was converged to, the solid and liquid phases would be considered simultaneously. This time the converged temperature would be T_m, but the amount of liquid would be negative. Removing the liquid phase would then permit convergence to the correct temperature T_s'. For this type of a situation, such a "modus operandi" is uneconomical since it unnecessarily requires one extra solution of the equilibrium equations. A more economical procedure would be to require simultaneous consideration of solid and liquid only in the region of oscillatory behavior indicated by the cross hatching (fig. 1). It can be seen from figure 1 that oscillatory behavior will occur for a given entropy if either of these conditions is satisfied

$$T_m - T_l < T_s - T_l \tag{48a}$$

or

$$T_s - T_m < T_s - T_l \tag{48b}$$

When the iteration converges to T_l, inequality (48a) is used to estimate whether T_s will be greater than T_m. When the iteration converges to T_s, inequality (48b) is used to estimate whether T_l will be less than T_m. An approximate relation between T_s and T_l can be obtained by using the fact that the entropy difference between the temperature T_l on the $\overline{P_2P_5}$ curve and the temperature T_s on the $\overline{P_3P_6}$ curve is zero. The specific heats of the two equilibrium mixtures are $(c_p)_l$ at T_l and $(c_p)_s$ at T_s, respectively, while the entropies at the points P_2 and P_3 are s_l and s_s, respectively. Therefore, approximately

$$s(T_s) \cong s(T_l) + (c_p)_l \ln \frac{T_m}{T_l} - (s_l - s_s) + (c_p)_s \ln \frac{T_s}{T_m} \tag{49a}$$

and, as a result,

$$s(T_l) - s(T_s) = 0 \cong s_l - (c_p)_l \ln \frac{T_m}{T_l} - s_s + (c_p)_s \ln \frac{T_m}{T_s} \tag{49b}$$

The points P_2 and P_3 differ only in the fact that at P_2 all of the condensed phase is liquid, while at P_3 all of the condensed phase is solid. Let the molecular weight of the equilibrium mixture at T_m be M_m and the combined mole fraction of solid and liquid in the equilibrium mixture be x_m. If the heat of fusion per mole of condensed species is ΔH_m, then s_l and s_s are related by the expression

$$s_l = s_s + \frac{x_m \Delta H_m}{M_m T_m} \tag{50}$$

Substituting this expression into equation (49b) gives

$$\frac{x_m \Delta H_m}{M_m T_m} - (c_p)_l \ln \frac{T_m}{T_l} + (c_p)_s \ln \frac{T_m}{T_s} = 0 \tag{51}$$

At the temperature T_l, the quantities $(c_p)_s$, M_m, and x_m would be unknown. If, however, the difference between T_s and T_l is not too large, then $(c_p)_s$, M_m, and x_m can be approximated by their values at

T_l. Under these conditions, equation (51) can be solved to give

$$T_s = T_l \exp\left[\frac{x_l \, \Delta H_m}{M_l (c_p)_l T_m}\right] \tag{52}$$

where the subscript l indicates the quantities are to be evaluated at T_l. Substitution in equation (48a) gives as the condition of no oscillation

$$\frac{T_m}{T_l} < \exp\left[\frac{x_l \, \Delta H_m}{M_l (c_p)_l T_m}\right] \tag{53}$$

At a temperature T_s, a similar treatment gives the condition for no oscillation as:

$$\frac{T_m}{T_s} > \exp\left[- \frac{x_s \, \Delta H_m}{M_s (c_p)_s T_m}\right] \tag{54}$$

where the subscript s indicates quantities are evaluated at T_s.

There is one disadvantage connected with the use of either inequality (53) or (54) in a computer program; that is, it requires the computation of ΔH, M, c_p, and the mole fraction of the condensed species. However, it is possible to use inequalities (53) and (54) to estimate the width of the oscillatory region about T_m by using data in the vicinity of T_m. Thus, for example, applying inequality (53) to data corresponding to $P_c/P = 2.5$ and inequality (54) to data corresponding to $P_c/P = 3.5$ of table X and using 26 kilocalories as the heat of fusion for Al_2O_3 give $T_m/T_l < 1.0363$ and $T_m/T_s > 0.964$. These data imply that oscillation will not occur if $T_m - T_l > 81^\circ$ K and $T_s - T_m > 87^\circ$ K. Using data for a few other typical systems indicated that a satisfactory region would be 100° K on each side of T_m, and, therefore, this value was incorporated into the program. However, it is possible that a system could be encountered where this interval is insufficient to prevent oscillation. For such a system the interval would have to be widened.

With the technique just described, if a liquid phase is being considered and the resulting temperature is below the melting point, two possibilities exist. If the temperature is more than 100° K below the melting point, the solid phase will replace the liquid phase and the iteration will be restarted. If the resulting temperature is less than 100° K below the melting point, the solid will be included, the liquid phase retained, and the iteration restarted. After convergence with both phases considered, the resulting temperature will be the melting point. The iteration is finished if the amounts of both phases are positive. If, however, the liquid phase is negative, it is removed and the iteration is restarted. An analogous procedure is followed if the solid phase only is being considered and if the temperature is above the melting point.

Accidental Singularities

A peculiar type of singularity can occur in the equations for determining the equilibrium conditions in a system with condensed products. The conditions for its occurrence are so restrictive that it may be termed an accidental singularity. These conditions are:

(1) The state of the system must be specified by an assigned temperature and pressure.

(2) For an l-element system ($l > 1$) there must be $l - 1$ condensed species.

(3) For $l > 2$, at least $l - 1$ of the elements must appear in the condensed species.

(4) For $l = 2$, both elements must appear in the one condensed species.

These conditions are sufficient, but not necessary, to have the gaseous composition completely determined by the equilibrium equations for the condensed species and the pressure equation without recourse to the mass-balance relations. This can most readily be seen by examining the iteration equations (fig. 1) for the two-element case. When the aforementioned conditions are satisfied, the l mass-balance equations serve only to determine the mass variable A and the moles of the $l - 1$ condensed species. If the gas compositions $n_j (j = 1, 2, . . ., m)$ are known, the mass-balance equations

$$\sum_{j=m+1}^{m+l-1} a_{ij} n_j - b_i^o A = - \sum_{j=1}^{m} a_{ij} n_j \qquad (i = 1, 2, . . ., l) \qquad (55)$$

are a set of linear equations for the l variables: A and $n_j (j = m + 1, m + 2, . . ., m + l - 1)$. The equations do not possess a nontrivial solution if the determinant of the coefficient matrix vanishes; that is, if

$$\begin{vmatrix} a_{1,m+1} & a_{1,m+2} & \cdots & a_{1,m+l-1} & b_1^o \\ a_{2,m+1} & a_{2,m+2} & \cdots & a_{2,m+l-1} & b_2^o \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{l,m+1} & a_{l,m+2} & \cdots & a_{l,m+l-1} & b_l^o \end{vmatrix} = 0 \tag{56}$$

The determinant (eq. (56)) could vanish if the $[l \times (l - 1)]$ matrix of a_{ij}'s is of rank less than $l - 1$. This case is excluded from consideration. For the simple case $l = 2$, equation (56) reduces to

$$\frac{a_{1,m+1}}{a_{2,m+1}} = \frac{b_1^o}{b_2^o} \tag{57}$$

The significance of the criterion (eq. (56)) for the existence of a singularity can be seen immediately if it is realized that the determinant will vanish when it is possible to find a linear combination of the first $l - 1$ columns, which will equal the last column (in other words when the overall composition can be expressed in terms of the condensed products alone).

It must be emphasized that this type of problem is singular only if the thermodynamic state is specified by an assigned temperature and pressure. If the state is specified by an assigned pressure and either an enthalpy or entropy, then a solution can be obtained because the gas phase composition is no longer determined exclusively by the equilibrium constants for the condensed phase and the pressure equation. While the occurrence of such singularities is rare, they have been encountered. One such case is the stoichiometric lithium-oxygen system. An important product in this system is the stoichiometric liquid $Li_2O(l)$. This satisfies (eq. (57)) and hence corresponds to a singularity. Many other examples could be given, but this one example sufficiently illustrates the point. Because these singularities are so rare, a routine for recognizing the situation and taking corrective measures was not incorporated into the program.

Assigned Pressures Too Low

In an all gaseous system, a pressure can be assigned to the system quite arbitrarily. However, in a system with condensed products, the assigned pressure can no longer be specified with complete freedom. The assigned pressure must be greater than the sum of the vapor pressures of the condensed species. The amount by which the assigned pressure must exceed the sum of the vapor pressures is determined by the partial pressures of other species in the gaseous phase. Should too low a pressure be assigned, the iteration will not converge since this would require that some of the partial pressures become negative. Because the corrections are logarithmic, a negative partial pressure cannot be obtained. Such a situation is characterized by large and negative $\Delta \ln n_j$ for some gases and small $\Delta \ln n_j$ for a few of the gases. The gases with small $\Delta \ln n_j$ are the vapors of the condensed species and those gases whose partial pressures can be expressed entirely in terms of equilibrium constants and the vapor pressures of the condensed species. The correction $\Delta \ln A$ is also large and negative. Again, because of the rarity of such a problem, no corrective measures have been incorporated into the program. The correct answer can be obtained by repeating the calculation with fewer condensed species present or by assigning a higher pressure.

THE COMPUTER PROGRAM

A computer program, based on the equations presented in the previous sections, was written for an IBM 704 computer with an 8K core, an 8K drum, and eight tape handlers. A detailed listing of this program is given in appendix C. The program has also been converted for use on an IBM 7090 computer with a 32K core and eight tape handlers. The 7090 program is given in appendix D.

The program can accommodate up to a 15-element system with 90 products of reaction and a maximum of 20 iteration equations. These limits on the size of the system that can be accommodated are dictated primarily by the IBM 704 core capacity. For the IBM 7090, the program can be readily altered to handle a larger system. At present, the program does not handle ionized species although provision has been made in Subroutine SEARCH for future consideration of ionized species.

The computer program can handle any one of five different problems. Each of these five calculations has been given an alphabetic code name with some mnemonic significance. Thus, an H,S problem is a rocket-performance calculation where the combustion is at an assigned enthalpy and pressure; this is followed by isentropic expansion, with composition in chemical equilibrium, to various exit pressures. The exit points are assigned in terms of pressure ratio P_c/P. A maximum of 25 pressure ratios may be specified including combustion pressure ratio $P_c/P = 1$ and throat pressure ratio. Since the program supplies its own estimate for the throat pressure ratio, a value of zero should be read in as the throat pressure ratio. The T,S problem differs from the H,S problem only in the fact that combustion is at an assigned temperature rather than at an assigned enthalpy. Both the H,S and the T,S problems include calculations for frozen composition during isentropic expansion. The T,P problem calculates equilibrium compositions for an assigned temperature and a series of up to 25 pressures. The P,T problem calculates equilibrium compositions for an assigned pressure and a series of temperatures not exceeding 25 in number. The DETN problem determines Chapman-Jouguet detonation properties for an assigned temperature and pressure preceding the detonation wave.

If, for some reason, it is desired to terminate the problem before the entire schedule of points has been completed, this can be done with sense switch 6. When sense switch 6 is in the down position, the problem will be continued for only one additional iteration for chemical composition. Intermediate output for this iteration will be written as well as the data for all completed points.

Because of the limited amount of core storage that was available on the IBM 704 computer, it was necessary to segment the problem into five core-loads, each with its own main program and subroutines. The five segments, or core-loads, are assumed to be available as five consecutive records comprising the first file on tape unit two. At the Lewis Research Center a computer monitoring system loads the core-loads onto tape two. These core-loads are then brought into core storage from tape two in any arbitrary sequence by the call statement CALL PONG (I) where I = 1, 2, . . ., 5. A program for loading the core-loads onto tape two will not be supplied since most computing centers will already have some system for doing this operation. The subroutine for calling core-loads also will not be supplied, and its function must be performed by an analogous subroutine available at the respective computing centers. The coding for the IBM 704 program is partially in FORTRAN II and partially in the pseudo-SAP of FORTRAN III.

The 7090 version of the program is essentially identical to the 704 version, except that because of the much larger core storage it was unnecessary to segment the program. In the program for the 7090, the main program for core-load one is the main program for the entire computer program while the main programs for core-loads two, three, four, and five are subroutines. The elimination of program segmenting has the dual effect of (1) appreciably decreasing the computation time because of the elimination of a great deal of tape handling, and (2) somewhat simplifying the program. During the course of program conversion, all FORTRAN III pseudo-SAP coding was eliminated to obtain a program written exclusively in FORTRAN II. This was made possible because of the availability (at the Lewis Research Center) of four functions to perform shifting operations. These functions ALSF(N,X), ARSF(N,X), LLSF(N,X), and LRSF(N,X) are compiled into the object program as open subroutines and replace the machine language instructions ALS, ARS, LLS, and LRS, respectively. The first argument N specifies the number of places that the second argument X is to be shifted. The subroutines are compiled as:

CAL N

ARS 18

STA *+2

CAL X

(Appropriate shift instruction)

Either STO for non-Boolean statements

or SLW for Boolean statements

For non-Boolean statements N can be either a fixed-point variable or a fixed point constant, while X can be either a fixed- or floating-point unsubscripted variable or constant. For Boolean statements N must be either a fixed-point variable or a Boolean constant whose last six octal digits must be zeros (e.g., 6000000), while X must be a floating-point unsubscripted variable or constant. see errata

The description of the program in the following sections and in the flow charts (figs. 2 to 9) will be confined to the IBM 704 version because the two programs are virtually identical. Since 80 card columns of input are used, input to both programs must be by means of an IBM 1401 or other card-to-tape equipment that will put all 80 card columns on tape. Under certain circumstances, the input may be through a card reader; this will be discussed further in the section PROGRAM INPUT DATA.

The source program decks for either the IBM 704 or IBM 7090 will be made available to computing centers if a written request is addressed to the authors at the Lewis Research Center. The thermodynamic data of appendix B will be furnished for program checkout purposes if a written request is made. The data will be supplied in the form of 23 word records (see fig. 6) copied onto a tape furnished by the computing center making the request. Because of continuous reevaluation of thermodynamic data, the data in appendix B will differ somewhat from the data in current use by the thermodynamics section for performance calculations. Current data will be furnished, upon request, in the same form as the data used for program checkout purposes.

see errata for additional paragraph.

Core-Load One

Core-load one consists of MAIN PROGRAM ONE (fig. 2) and the three Subroutines INPUT, SEARCH, (fig. 6) and BYPASS (fig. 7). The principal function of this core-load is to process input information. This portion of the program (1) assembles thermodynamic data from the master data tape, (2) determines which species shall be used in the calculation, (3) determines which of the five types of problems is to be worked, and (4) calculates the overall system composition from the assigned value of any one of the three quantities: O/F, %F, or $\mathcal{R}$.

Subroutine INPUT. - Subroutine INPUT processes the input information on the reactant cards, which contain the formulas of the fuels or oxidants, their enthalpies, and densities. From this information the subroutine calculates the gram-atoms of each element per gram of effective fuel, the gram-atoms of each element per gram of effective oxidant, and the corresponding enthalpies (see eqs. (21) and (23)). In addition to the various gram-atoms and enthalpies per gram, the positive and negative oxidation states per gram are also calculated (see eqs. (26) to (29)).

The densities of the effective fuel and oxidant are calculated by Subroutine INPUT except in the case of a detonation problem. For detonation problems, the specific heats of the reactants must be read into the computer in place of the densities. These are used to calculate $(c_p)_f$, which in turn is used in the evaluation of detonation derivatives with respect to T_1 (see table VI).

In order for Subroutine INPUT to perform the aforementioned calculations, a table of symbols, atomic weights, and oxidation states for the chemical elements is needed. This table is read into storage by calling the Subroutine BCREAD(A,B), which reads a set of absolute binary cards into ATOM(I,J). The element symbols are in ATOM(I,1), the atomic weights are in ATOM(I,2), and the oxidation states are in ATOM(I,3). Since the index I can range from 1 to 103, there is space for 103 different chemical elements. The symbols for the chemical elements must be in binary coded decimal and left-adjusted (e.g., AL0000, Hb0000), while the atomic weights and oxidation states must be floating point-numbers. The oxidation states are those which correspond to the most common oxidation states of the elements (e.g., aluminum, +3.0; sulfur, +4.0; chlorine, -1.0). Subroutine BCREAD is a part of the computer system at the Lewis Research Center and is not given in this report. Any subroutine or sequence of statements that will read the element data into ATOM(I,J) can be substituted for subroutine BCREAD. The element data in ATOM(I,J) are considered constants of the program rather than input data (see section PROGRAM INPUT DATA), inasmuch as they are constant for all problems.

Subroutine SEARCH. - Subroutine SEARCH selects the thermodynamic data to be used in the problem. A scan is made of the master thermodynamic data tape; those species that are consistent with the chemical system under consideration are selected. These are written as a separate file on the master data tape. As the thermodynamic data are being selected, the subroutine also compiles a set of formula numbers a_{ij} from the formulas of the reaction products.

Subroutine BYPASS. - Subroutine BYPASS interrogates or alters any one of 90 bit positions in one of the three words PROD(1), PROD(2), or PROD(3). Each bit position is associated with a particular reaction product. A reaction product is considered in the calculation only if its corresponding bit position is zero. The first argument (J) of the subroutine specifies a particular bit position, while the second (IARG) determines the function to be performed by the subroutine. If IARG =1, BYPASS interrogates bit position J, setting IPROD to 2 if the bit is 0 or setting IPROD to 1 if it is nonzero. When IARG = 2, BYPASS changes the appropriate bit from a 0 to a 1, while for IARG = 3 BYPASS changes a 1 to 0.

Core-Load Two

MAIN PROGRAM TWO (fig. 3) and the Subroutines BYPASS (fig. 7), MATRIX (fig. 8), and GAUSS (fig. 9) comprise core-load two. All computations of the equilibrium compositions of complex mixtures are performed in this core-load. In addition, for H,S and T,S problems, this core-load also calculates equilibrium rocket performance parameters.

Subroutine BYPASS. - Subroutine BYPASS is described under core-load one.

Subroutine MATRIX. - Subroutine MATRIX's sole function is the construction of the iteration equations (see table I) appropriate to the current problem.

Subroutine GAUSS. - Subroutine GAUSS is used to solve the set of simultaneous, linear iteration equations constructed by Subroutine MATRIX. The solution is effected by performing a Gauss reduction using a modified pivot technique. In this modified pivot technique only rows are interchanged. The row to be used for the elimination of a variable is selected on the basis that the largest of its elements, after division by the leading element, must be smaller than the largest element of the other rows after division by their leading elements.

An iterative feature has been incorporated into Subroutine GAUSS. A correction to the solution is obtained by replacing the right-hand side of the equation by the residuals, that is, by the difference between the right-hand side and the value of the right-hand side as calculated from the solution. This set of equations is now re-solved for corrections to the previous solution. Iteration is continued until no further improvement in the solution is possible or for a maximum of four iterations. The criterion for improvement of a solution is the decrease of a test function defined to be the sum of the magnitudes of the fractional residuals for those equations whose right-hand sides are greater than 1 in magnitude plus the sum of the magnitudes of the residuals of the remaining equations.

Core-Load Three

The evaluation of rocket performance parameters for isentropic expansion with composition frozen at the equilibrium composition in the combustion chamber is done in MAIN PROGRAM THREE (fig. 4). There are no subroutines for this core load.

Core-Load Four

Core-load four does the calculations required to obtain Chapman-Jouguet detonation properties and prints the results in a suitable form. A flow chart for MAIN PROGRAM FOUR is given in figure 5. Flow charts for the Subroutines OUT, COMP, ONCE, and SPEC are not given since these only print the answers in a convenient form.

Core-Load Five

The last core-load is an output program; that is, it merely takes the results of calculations for H,S; T,S; T,P; and P,T problems and prints them in a convenient form. No flow chart is given for this program.

PROGRAM INPUT DATA

A number of options are available in the program. These options include the following:

(1) Selection of any of five types of problems

(2) Omission of any gaseous reaction product

(3) Initial consideration of any condensed reaction product

Because of these options, the input to the program, although simple and straightforward, is larger than it need be for a less flexible program.

In addition to blank cards, five types of input cards are needed to supply all of the required information to the program (see discussion of element data in section Subroutine INPUT). These five types of cards are given in the appropriate order in table VIII. Blank cards are used after each input card type whose number is variable. Upon encountering a blank card the program will terminate the reading of one card type and will begin reading the next card type in the input sequence. A description of the nonblank cards is given below.

Reactant Cards

Table IX gives three sets of reactant cards. The first set corresponds to a typical solid propellant, the second is typical of the set of reactants for a liquid or gaseous propellant, and the third is a typical set for a detonation calculation. In particular, these three sets of reactant cards are those used in the calculations of tables X to XV.

The format selected for these cards was based on ease of specifying the reactants for either gaseous, liquid, or solid propellants. For liquid or gaseous propellants the reactants are generally categorized as fuels or oxidants. An F keypunched into column 72 indicates that the substance is a fuel, while an O signifies an oxidant. When more than one fuel is used, the program combines the fuels into an effective fuel if the relative weight of each fuel is given in columns 46 to 53 (a decimal point must be given). If only one fuel is used, then any number (with a decimal point) may be placed into columns 46 to 53. A similar description covers the case where the propellant contains one or more oxidants.

For solid propellants, the reactants are usually not labeled as either fuels or oxidants. The composition of the solid propellant is normally given in terms of the relative weights of each ingredient. However, for input purposes each ingredient of a solid propellant is designated as a fuel (i.e., F in column 72). Since all ingredients are considered as components of a fuel, 100-percent fuel must be specified on the mixture card (see below).

The chemical formula for the reactant appears in columns 1 to 45 and may contain up to five different chemical elements per reactant. Each chemical symbol is allowed two columns (left-adjusted for a one-symbol element). Each formula number is allowed up to six figures plus a decimal point. The decimal point is required even for integers.

The state of the reactants (S, L, or G in column 63) and their temperature (columns 64 to 71) are for information purposes only. They may be omitted if desired since this information is not required by the program. The enthalpies of the reactants are given in columns 54 to 62, which supply enough space for eight digits and a decimal point if the number is positive or seven digits, a sign, and a decimal point if the number is negative. The enthalpy values must be consistent with the enthalpy base selected for the thermodynamic data (see the discussion in the section Thermodynamic Data). These enthalpies are used in equation (23) to calculate h_x and h_f, which are then used in equation (24) to calculate assigned enthalpies for H,S problems. For the H,S; T,S; T,P; and P,T type problems, columns 73 to 80 are reserved for the densities of the reactants. Space has been provided for seven digits and a decimal point. If the densities of all reactants are given, the density of the propellant mixture will be calculated; otherwise the propellant density is printed as zero in the output. For a DETN type problem, columns 73 to 80 must contain the heat capacity at constant pressure for the reactant.

If an on-line card reader is used to read the input data instead of an IBM 1401, the contents of columns 73 to 80 will not be read. For the H,S; T,S; P,T; and T,P problems, all calculations will be unaffected (and a value of zero will be printed on the output format for the density of the unreacted mixture). For the DETN problem, all answers will be correct except for detonation derivatives with respect to T_1 and the following functions of the unreacted mixture: isentropic exponent, sonic velocity, and Mach number of the detonation wave.

Omit-Insert Cards

Subroutine SEARCH, previously described, selects from the master thermodynamic tape all species that are consistent with a given chemical system. In the absence of prior information the program makes the initial assumption that all the selected gaseous species may exist in appreciable concentrations and that condensed species will not be present, at least for the equilibrium conditions corresponding to the first point. When the iteration converges, the latter assumption is checked and, if necessary, corrected automatically.

Omit-Insert cards serve two different purposes depending on whether the formula for a gaseous or condensed species appears on the card. If the formula for a gaseous species is on the card, that species will not be considered by the program for all assigned conditions. This permits the omission of any gaseous species from the calculation without the necessity of remaking the master thermodynamic data tape. The omission of one or more gaseous species may be desired in order to determine the resulting effect on composition or other properties of the system. The omission of gaseous species may sometimes also be desired in order to reduce calculating time. (This assumes some "a priori" knowledge of which species may be omitted without affecting the results to the desired number of significant figures.) If the formula for a condensed species is on the Omit-Insert card, the program will initially consider this species to be present at the assigned conditions corresponding to the first point. After convergence, this assumption is checked automatically and corrected if necessary. In contrast to gaseous species, a condensed species can be omitted from consideration by the program only by removing it from the master thermodynamic tape.

The names of up to four species can appear on each Omit-Insert card in columns 1 to 12, 16 to 27, 31 to 42, and 46 to 57. The names must be keypunched exactly as they appear on the master thermodynamic tape (appendix B).

Problem Cards

These cards are used to specify which one of the five problems is to be worked (H,S; T,S; P,T; T,P; or DETN) and also to assign an identifying case number to the problem. Columns 1 to 4 contain the alphabetic designation for the problem beginning in column 1. The assigned case number is a set of five digits keypunched into columns 6 to 10. This case number appears on the output listing.

Schedule Cards

Every type of problem except DETN requires a schedule of points to be calculated. For the DETN problem the schedule cards and the blank card that follows them must be omitted while the other input cards remain as before. The schedule for the other four problems must not exceed 25 points. For the H,S and T,S problems the schedule of points is a series of pressure ratios P_c/P. The first pressure ratio (combustion chamber) must be unity; the second, corresponding to throat, is left blank; and all others are optional. For the T,P problem, the schedule is a series of 25 or less assigned pressures in atmospheres. For the P,T problem the schedule is a series of 25 or less assigned temperatures in $^{\circ}K$.

Each schedule card contains as many as five assigned values in columns 1 to 10, 11 to 20, 21 to 30, 31 to 40, and 41 to 50. Thus there is enough space for nine digits and the required decimal point for each assigned value.

Mixture Cards

The mixture card is used to specify the relative amounts of the effective fuel and oxidant and to provide either initial estimates or assigned values for pressure and temperature. In addition, the mixture card permits two options. The first option permits intermediate output to be printed for each composition iteration if an integer is keypunched in column 72. The intermediate output is described in the section INTERMEDIATE OUTPUT. The second option may be used only in the DETN problem. If the code columns (i.e., columns 51 to 55) are left blank, the sonic velocity of the burned gas is calculated by use of γ; if they are nonblank (any integer with no decimal point), then the sonic velocity is calculated from κ, the ratio of equilibrium specific heats.

The relative amount of fuel and oxidant is specified by any one of the three quantities $\mathfrak{R}$, O/F, or %F; the card columns corresponding to the remaining two are left blank. Columns 1 to 10, 11 to 20, and 21 to 30 are for $\mathfrak{R}$, O/F, %F, respectively. In each case, there is sufficient space for nine digits plus a required decimal point. Columns 31 to 40 and 41 to 50 provide space for a pressure and temperature, respectively. The purpose of the pressure and temperature differs from problem to problem. For the H,S problem the pressure in pounds per square inch absolute is the assigned combustion pressure, while the temperature in $^{\circ}$K is the estimate for combustion temperature. For this problem the temperature is optional. If the temperature is left blank, the program automatically uses a temperature estimate approximately equal to 3800° K. For a T,S problem, the pressure in pounds per square inch absolute is the combustion pressure and the temperature in $^{\circ}$K is taken to be the combustion temperature. For the T,P problem the pressure is ignored by the program, while the temperature in $^{\circ}$K is the assigned temperature for the series of pressures read in on the schedule card. For the P,T problem the pressure in atmospheres is the assigned pressure for the series of temperatures read in on the schedule card, while the temperature on the mixture card is ignored. In the DETN problem, the pressure in atmospheres and the temperature in $^{\circ}$K correspond to the pressure and temperature preceding the detonation wave.

PROGRAM OUTPUT

Tables X to XIII are examples of the final output for three types of problems. Tables X and XI are the output of an H,S problem for a solid propellant. Table XII is the output of a P,T problem for stoichiometric hydrogen-air. Table XIII is the output of a Chapman-Jouguet detonation calculation (DETN) for stoichiometric hydrogen-oxygen.

The three tables are almost completely self-explanatory; however, the symbols for some quantities are somewhat different than those used in the text. The reason for this is that the IBM printer does not contain characters such as lower-case letters, Greek letters, subscripts, or superscripts. The following examples illustrate the differences:

$$(DLI/DLPC)PC/P = (\partial \ln I/\partial \ln P_c)P_c/P, h_c$$

$$(DLCS/DHC)PC/P = (\partial \ln c^*/\partial h_c)P_c/P, P_c$$

$$(DLAR/DLPCP)S = (\partial \ln \epsilon/\partial \ln P_c/P)_s$$

During the calculation of the data of table X, the program considered the possible occurrence of 11 condensed species (counting solid and liquid phases of the same species separately). Of these 11 only four appeared in nonzero amounts, namely, $MgO(s)$, $MgCl_2(s)$, $Al_2O_3(s)$, and $Al_2O_3(l)$. Of these four species, only $Al_2O_3(l)$ was keypunched into an Omit-Insert card for initial consideration by the program; the other three species were put into the calculation, at the appropriate time, by the program. Furthermore, $MgO(s)$ and $Al_2O_3(l)$ were removed from the calculation based on decisions made by the program. Points four, five, and six of table X illustrate the typical behavior when two condensed forms of the same species coexist. In this example, the coexisting species are $Al_2O_3(l)$ and $Al_2O_3(s)$ and the temperature for these points is the melting point of $Al_2O_3(s)$. For these same three points, the molecular weight derivatives appear as zero. The reason for this is that the equations of tables II and III are singular for the coexistence of two forms of the same condensed species. This prevents the calculation of the molecular weight derivatives and the heat capacity at constant pressure. However, for the purpose of calculating a velocity of sound it was felt desirable to calculate a frozen heat capacity at constant pressure, which could then be used to calculate a frozen isentropic exponent. As a final point, it should be noted that the program lists separately those species that were considered in the calculation but which were only present in trace amounts and those species that were intentionally omitted from the calculation because their formulas were keypunched on Omit-Insert cards.

In table XI only four points are listed although the same points that were calculated in the equilibrium calculation of table X were specified in the frozen calculations. The reason for this is that in the frozen program the calculation is terminated when a sufficiently low temperature is reached so that a species, present at combustion, no longer has thermodynamic data at this temperature. In table XI the species $Al_2O_3(l)$ has data only to the melting temperature 2317° K. Since the program permits extrapolations for 20° beyond the end point, the program considers that data for $Al_2O_3(l)$ exist to 2297° K. The presence of the last point at a temperature of 2270° K can be accounted for because the program permits completion of the calculation for the first point past the 20° extrapolation limit.

The program can list the reactant input data in one of two format types. The first of these is used when at least one of the reactants has a noninteger formula number. This type is illustrated in tables X, XI, and XII. The second format is reserved for those systems where all formula numbers are integers. This is illustrated in table XIII.

The preliminary output (table XIV) is written primarily to provide information as to what problem the program is working in the event no final output is obtained. The last line of table XIV is printed during frozen expansion in the event that the exit temperature is below the temperature range of a species (see discussion of table XI).

INTERMEDIATE OUTPUT

Many safety features have been incorporated into the program that will prevent the calculation from becoming divergent. However, it was not possible to include corrective measures for two situations. The first is the problem of poorly conditioned iteration equations whose solution results in excessive fractional residuals ($>0.5\times10^{-4}$). The second is the problem of singular iteration equations. In these two situations the program returns to the first iteration for the initial point and begins iterating, this time printing intermediate output to assist in debugging. Table XV is the debug output from the solid propellant calculations shown in tables X and XI. This output was obtained by the method described in the section Mixture Cards, rather than resulting from either of the two situations just discussed.

All of the legends that appear on the right-hand side of table XV(a) are not written by the program. Similarly the headings in table XV(b) have also been typed. In table XV(a) the first line gives the case number assigned to the problem and the type of problem; the second line gives O/F, $\%F$, $\Re$, and P_c; the third and fourth lines give the enthalpy per gram of propellant h_0 and the gram-atoms of the elements per gram of propellant b_i^o, which for this problem are b_N^o, b_H^o, b_{Cl}^o, b_O^o, b_C^o, b_S^o, b_{Al}^o, and b_{Mg}^o. The next 22 lines are the iteration equations corresponding to table I. For some problems each iteration equation requires only one line. However, for this example, each equation of table I requires two lines. The first 16 of these 22 lines correspond to eight reduced mass-balance equations for the eight elements in this problem which have been taken in the following order: nitrogen (N), hydrogen (H), chlorine (Cl), oxygen (O), carbon (C), sulfur (S), aluminum (Al), and magnesium (Mg). The next two lines are for $Al_2O_3(l)$. The last four lines are for the pressure and enthalpy equations. For this problem, the coefficients of $\Delta \ln u_k$, $\Delta n_{Al_2O_3(l)}$, $-\Delta \ln A$, $\Delta \ln T$, and the right-hand side of each equation are given by the eight columns of line one and the first four columns of line two for each pair of lines. The fifth column of line two gives the fractional residuals for that equation (see discussion of fractional residuals in the section on Subroutine GAUSS).

In table XV(a) following the set of iteration equations are two lines which give the solution to the preceding set of iteration equations. The next line gives the current value of T, P, A, and λ. The remaining 81 lines give the formulas, n_i, $\ln n_i$, $\Delta \ln n_i$ (or Δn_i for condensed species), $\mathcal{H}_i$ and $\mathcal{S}_i$ for each of the 81 species. The word OMIT preceding the formula for a species indicates that this product is not considered as a product of reaction for this problem. It may be noted that the initial estimate is 1 atmosphere for each gaseous species and zero moles for each condensed species. A zero in the Δn_i column for a condensed reaction product indicates that this species is not being considered during the iteration. It should also be noted that the correction to $Al_2O_3(l)$ is negative, and, therefore, $Al_2O_3(l)$ will be present in negative amount during the second iteration although when the iteration converges it will be positive. This indicates the inadvisability of checking the condensed species at each stage of the iteration. A final point to note is that λ for this iteration was determined by the species CO(g).

The previous sequence of lines is printed for each iteration. When the iteration converges, the answers are printed as shown in table XV(b). This set of answers corresponds to the throat pressure ratio $P_c/P = 1.777$ of the data of table VIII.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, June 26, 1962

APPENDIX A

SYMBOLS

A	total mass reactant
A/w	nozzle area per unit mass-flow rate
$(A/w)_t$	area per unit mass-flow rate at nozzle throat
a_{ij}	formula numbers giving gram-atoms of i^{th} element in j^{th} species
a_{ij}^x, a_{ij}^f	formula numbers of oxidants and fuels giving gram-atoms of i^{th} element in j^{th} oxidant and fuel, respectively
$a_1, a_2, \ldots, a_7$	constants in empirical equations for thermodynamic data
b_i	gram-atoms of i^{th} element per unit mass of mixture, $\frac{1}{A}\sum_{j=1}^{n} a_{ij}n_j$
Δb_i	$b_i^o - b_i$
b_i^o	assigned value for gram-atoms of i^{th} element per unit mass of reactant
$(b_x^o)_i, (b_f^o)_i$	gram-atoms of i^{th} element per gram of effective oxidant or effective fuel
C_F	thrust coefficient
$(C_p^o)_j$	heat capacity of j^{th} species at constant pressure per mole, $\left[\frac{\partial(H_T^o)_j}{\partial T}\right]_P = T\left[\frac{\partial(S_T^o)_j}{\partial T}\right]_P$
$\mathscr{C}_j$	heat capacity per mole at constant pressure for j^{th} species divided by gas constant, $\frac{(C_p^o)_j}{R}$

c_p	heat capacity of reaction products at constant pressure per unit mass
$(c_p)_f$	frozen heat capacity of the unreacted mixture at constant pressure per unit mass evaluated at T_1
$(c_p)_l, (c_p)_s$	heat capacity of reaction products at constant pressure per unit mass evaluated at T_l and T_s, respectively
c_v	heat capacity of reaction products at constant volume per unit mass
$c*$	characteristic velocity
$(F_T^o)_j$	standard-state free energy per mole of j^{th} species, $(H_T^o)_j - T(S_T^o)_j$
%F	weight or mass percent fuel
$\mathscr{F}_j$	free energy per mole of j^{th} species divided by RT, $\frac{(F_T^o)_j}{RT} + \ln n_j \quad (j = 1, 2, . . ., m)$ and $\frac{(F_T^o)_j}{RT} \quad (j = m + 1, m + 2, . . ., n)$
g_c	gravitational conversion factor, 32.174 (lb mass/lb force)(ft/sec^2)
ΔH_m	heat of fusion per mole of condensed species
$(H_T^o)_j$	enthalpy per mole of j^{th} species
$\mathscr{H}_j$	enthalpy per mole of j^{th} species divided by RT, $\frac{(H_T^o)_j}{RT}$
h	enthalpy of reaction products per unit mass of reactant, $\frac{1}{A}\sum_{j=1}^{n} (H_T^o)_j n_j$
h_c	combustion enthalpy of reaction products per unit mass of reactant

h_0	assigned enthalpy per unit mass of reactant
h_1	enthalpy per unit mass of reactant before detonation wave
h^*	throat iteration parameter, $h + \frac{\gamma RT}{2M}$
$\mathcal{h}$	enthalpy of reaction products per unit mass of reactant divided by RT, h/RT
$\Delta \mathcal{h}$	$\mathcal{h}_0 - \mathcal{h}$
$\mathcal{h}_0$	assigned enthalpy per unit mass of reactant divided by RT, h_0/RT
I	specific impulse with ambient and exit pressures equal, (lb force)(sec)/lb mass
I_{vac}	specific impulse into vacuum (ambient pressure equal to zero), (lb force)(sec)/lb mass
l	number of different chemical elements
M	molecular weight, A/P
M_c	combustion-chamber molecular weight
M_i^x, M_i^f	formula weights of i^{th} oxidant and i^{th} fuel
M_l, M_m, M_s	molecular weight at T_l, T_m, and T_s, respectively
M_1	molecular weight of gas before detonation wave
$\mathcal{M}$	Mach number, U/U_s
m	number of gaseous reaction products
n	total number of reaction products
n_j	moles of j^{th} species
O/F	oxidant-to-fuel weight or mass ratio
P	static pressure, atm
ΔP	$P_0 - P$
P_c	combustion pressure, atm

P_0 assigned static pressure, atm

P_1 pressure before detonation wave, atm

p_j partial pressure of j^{th} species, atm

R universal gas constant, 1.98726 cal/(mole)($^{\circ}$K)

$\Re$ equivalence ratio, $-[V_f^+ + (O/F)V_x^+]/[V_f^- + (O/F)V_x^-]$

r density ratio across a shock, ρ/ρ_1

r_{ik} $= r_{ki} = \sum_{j=1}^{m} a_{ij}a_{kj}n_j$

$(S_T^o)_j$ entropy per mole of j^{th} species in standard state

$\mathscr{S}_f$ $\sum_{i=1}^{n} x_i \frac{(S_T^o)_i}{R} - \sum_{i=1}^{m} x_i \ln x_i + \ln \frac{P_c}{P} \sum_{i=1}^{m} x_i$

$\mathscr{S}_f^o$ $\left(\frac{s_c M_c}{R} + \ln \frac{P_c}{\sum_{i=1}^{m} x_i}\right) \sum_{i=1}^{m} x_i$

$\mathscr{S}_j$ entropy per mole of j^{th} species divided by R,

$$\frac{(S_T^o)_j}{R} - \ln n_j \qquad (j = 1, 2, \ldots, m) \text{ and}$$

$$\frac{(S_T^o)_j}{R} \qquad (j = m + 1, m + 2, \ldots, n)$$

s entropy per unit mass of reactant

s_c combustion entropy per unit mass of reactant

s_l, s_s entropy per unit mass of reactant at T_l and T_s, respectively

s_0 — assigned entropy per unit mass of reactant (taken to be equal to s_c)

$\mathscr{s}$ — entropy per unit mass of reactant divided by R,

$$\frac{s}{R} = \frac{1}{A} \sum_{j=1}^{n} \mathscr{s}_j n_j$$

$\Delta\mathscr{s}$ — $\mathscr{s}_0 - \mathscr{s}$

$\mathscr{s}_0$ — assigned entropy per unit mass of reactant divided by R, s_0/R

T — absolute temperature

T_c — combustion chamber temperature

T_l, T_m, T_s — equilibrium temperature for assigned entropy and pressure where condensed species is all liquid, mixture of liquid and solid, or all solid, respectively

T_1 — absolute temperature before detonation wave

U — flow velocity

U_D — detonation velocity

U_s — sound velocity, $\sqrt{(\partial P/\partial \rho)_s}$

$\Delta \ln u_k$ — k^{th} component of solution vector of iteration equations in table I where $k = 1, 2, \ldots, l$

V_i^+, V_i^- — positive and negative oxidation states of an element in its commonly occurring compounds

W_i^x, W_i^f — weight of i^{th} oxidant or i^{th} fuel

w — mass-flow rate, lb mass/sec

x_j — mole fraction of j^{th} species in mixture

x_l, x_m, x_s — mole fraction of condensed species at T_l, T_m, and T_s, respectively

α_k — $\left(\frac{T_1}{T}\right)_k \frac{M}{M_1}$

γ isentropic exponent, $(\partial \ln P/\partial \ln \rho)_s$

γ_c isentropic exponent in combustion chamber

ϵ area ratio

κ c_p/c_v

Λ any parameter

λ empirical parameter $(0 < \lambda \leq 1)$ used to control size of corrections during iteration, defined in eq. (42)

λ_1, λ_2 convergence parameters defined in eqs. (40) and (41), respectively

ρ density

APPENDIX B

THERMODYNAMIC DATA

Formula		Temperature range for which data exists						
First temperature interval		a_1	a_2	a_3	a_4	a_5	a_6	a_7
Second temperature interval		a_1	a_2	a_3	a_4	a_5	a_6	a_7
AL1(G)		300.00	5000.00					
1000.	5000.	2.5378209E 00	-6.0990708E-05	3.9335798E-08	-1.1559831E-11	1.2920262E-15	3.8209820E 04	5.3500915E 00
300.	1000.	2.8352368E 00	-1.5134012E-03	2.7183744E-06	-2.2060285E-09	6.7171701E-13	3.8160129E 04	3.9723901E 00
AL1(L)		932.00	5000.00					
1000.	5000.	3.5224379E 00	-0.	-0.	-0.	-0.	1.6656099E 02	-1.5508453E 01
300.	1000.	3.5224379E 00	-0.	-0.	-0.	-0.	1.6656099E 02	-1.5508453E 01
AL1(S)		300.00	932.00					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	2.3894182E 00	2.2240533E-03	-1.9377647E-06	2.1410140E-09	-8.4670972E-13	-7.9799765E 02	-1.0797954E 01
AL2(G)		300.00	5000.00					
1000.	5000.	4.3671430E 00	3.0532349E-04	-1.3159070E-07	3.3852618E-11	-2.5891547E-15	5.7515589E 04	1.9181777E 00
300.	1000.	3.6400942E 00	3.8082887E-03	-6.5342309E-06	5.2533020E-09	-1.5953154E-12	5.7639052E 04	5.2971737E 00
AL1CL1(G)		300.00	5000.00					
1000.	5000.	4.3435193E 00	2.4626925E-04	-8.0780977E-08	1.2587611E-11	-1.7478140E-16	-7.0265398E 03	2.5080407E 00
300.	1000.	3.1509669E 00	5.6985381E-03	-9.7632780E-06	7.8095008E-09	-2.3742884E-12	-6.8070185E 03	8.1294577E 00
AL1CL3(G)		300.00	5000.00					
1000.	5000.	9.4205658E 00	6.5940434E-04	-2.9058869E-07	5.6462274E-11	-4.0336916E-15	-7.2876725E 04	-1.6346444E 01
300.	1000.	5.0572488E 00	1.9927263E-02	-3.3537735E-05	2.6197755E-08	-7.8027250E-12	-7.2040540E 04	4.3859034E 00
AL1F1(G)		300.00	5000.00					
1000.	5000.	4.1250002E 00	4.7152930E-04	-1.8874659E-07	3.6937215E-11	-2.6595077E-15	-3.2168337E 04	2.0564913E 00
300.	1000.	2.6936710E 00	5.7333440E-03	-7.6849735E-06	4.9038110E-09	-1.2037923E-12	-3.1845665E 04	9.1080542E 00
AL1F3(G)		300.00	5000.00					
1000.	5000.	8.5682068E 00	1.6264060E-03	-7.1915113E-07	1.4050250E-10	-1.0099185E-14	-1.4621756E 05	-1.7013311E 01
300.	1000.	2.3231444E 00	2.6091341E-02	-3.8375822E-05	2.6854646E-08	-7.2874477E-12	-1.4487581E 05	1.3404073E 01
AL1F3(S)		300.00	727.00					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	-1.1651746E 00	6.3861994E-02	-1.3953832E-04	1.5222939E-07	-6.2728634E-11	-1.8082155E 05	5.7075114E-01
AL1F3(S)		727.00	1551.70					
1000.	5000.	1.0532089E 01	1.5096162E-03	-0.	-0.	-0.	-1.8256162E 05	-5.2826117E 01
300.	1000.	1.0532089E 01	1.5096162E-03	-0.	-0.	-0.	-1.8256162E 05	-5.2826117E 01
AL1H1(G)		300.00	5000.00					
1000.	5000.	3.3055232E 00	1.3458802E-03	-5.3535427E-07	1.0142734E-10	-7.1297971E-15	2.9881497E 04	3.2542706E 00
300.	1000.	3.7716542E 00	-2.7674967E-03	8.7990133E-06	-8.1865699E-09	2.5937470E-12	2.9912423E 04	1.5929917E 00
AL1O1(G)		300.00	5000.00					
1000.	5000.	3.9517542E 00	6.7161259E-04	-2.8263938E-07	5.5049053E-11	-3.6818788E-15	7.1749763E 03	3.3586492E 00
300.	1000.	2.8420587E 00	3.7688103E-03	-3.0275652E-06	5.9586224E-10	2.1292872E-13	7.4725229E 03	9.0649964E 00
AL2O1(G)		300.00	5000.00					
1000.	5000.	5.7717507E 00	1.3771553E-03	-6.0307233E-07	1.1694669E-10	-8.3563570E-15	-2.1806545E 04	-2.7312889E 00
300.	1000.	2.5425147E 00	1.1856117E-02	-1.3328517E-05	6.8442771E-09	-1.2599683E-12	-2.1006485E 04	1.3529702E 01
AL2O2(G)		300.00	5000.00					
1000.	5000.	8.5025524E 00	2.2358185E-03	-9.7926896E-07	1.9006350E-10	-1.3595570E-14	-5.5983474E 04	-1.8757581E 01
300.	1000.	2.9710403E 00	2.2334000E-02	-2.9909695E-05	1.9675020E-08	-5.1347976E-12	-5.4704576E 04	8.6050963E 00
AL2O3(L)		2317.00	5000.00					
1000.	5000.	1.7612190E 01	-0.	-0.	-0.	-0.	-1.9925561E 05	-9.6060673E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
AL2O3(S)		300.00	2317.00					
1000.	5000.	9.1785079E 00	1.1460618E-02	-7.8355820E-06	2.5056206E-09	-3.1153252E-13	-2.0496297E 05	-5.0027668E 01
300.	1000.	-4.9920865E 00	8.0006637E-02	-1.3428568E-04	1.0711676E-07	-3.2848219E-11	-2.0256090E 05	1.5801944E 01
AL1O1CL1(G)		300.00	5000.00					
1000.	5000.	6.7507573E 00	8.5787200E-04	-3.8191279E-07	7.[illegible]047782E-11	-5.4209511E-15	-4.9505540E 04	-9.1527385E 00
300.	1000.	2.7871112E 00	1.7363022E-02	-2.7400723E-05	2.0391301E-08	-5.8443709E-12	-4.8699473E 04	9.9190667E 00
AL1O1F1(G)		300.00	5000.00					
1000.	5000.	6.3993573E 00	1.2486650E-03	-5.5102929E-07	1.0742911E-10	-7.7066767E-15	-7.4145336E 04	-9.1831766E 00
300.	1000.	1.1376981E 00	2.2321712E-02	-3.3766878E-05	2.4246955E-08	-6.7427554E-12	-7.3036114E 04	1.6335228E 01
AR1(G)		300.00	5000.00					
1000.	5000.	2.4998921E 00	7.3440446E-08	-3.3705635E-11	1.0586262E-14	-1.2191864E-18	9.3976654E-02	4.3668417E 00
300.	1000.	2.4899911E 00	7.4950654E-05	-1.9402281E-07	2.0849707E-10	-7.9474831E-14	9.9251224E-01	4.4077258E 00
B1(G)		300.00	5000.00					
1000.	5000.	2.5029722E 00	-7.2796638E-06	6.7266744E-09	-2.6446144E-12	3.7018727E-16	6.4932567E 04	4.1828497E 00
300.	1000.	2.5091600E 00	-5.0370772E-05	1.0926182E-07	-1.0537852E-10	3.7472246E-14	6.4932010E 04	4.1568983E 00
B1(L)		2300.00	5000.00					
1000.	5000.	3.6733995E 00	-0.	-0.	-0.	-0.	8.9872494E 01	-2.1153170E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
B1(S)		300.00	2300.00					
1000.	5000.	6.8384367E-01	3.6040784E-03	-1.8416031E-06	3.9854954E-10	-2.2617850E-14	-1.7127029E 02	-4.1743641E 00
300.	1000.	-2.6769618E-01	9.3280007E-03	-1.6683605E-05	1.7788969E-08	-7.3434201E-12	-1.7802426E 01	1.2911252E-01
B2(G)		300.00	5000.00					
1000.	5000.	3.9064189E 00	7.0427690E-04	-2.8030770E-07	5.3475995E-11	-3.7666405E-15	9.7403159E 04	1.6082688E 00
300.	1000.	3.0060020E 00	2.3624124E-03	1.9357754E-07	-2.4138284E-09	1.2319348E-12	9.7686232E 04	6.4465602E 00
B1CL1(G)		300.00	5000.00					
1000.	5000.	4.0956886E 00	4.9957207E-04	-1.9663025E-07	3.7673670E-11	-2.6435798E-15	1.9302594E 04	1.9757198E 00
300.	1000.	2.6988825E 00	5.4300094E-03	-6.9028205E-06	4.1759555E-09	-9.6836672E-13	1.9628152E 04	8.9091747E 00
B1CL2(G)		300.00	5000.00					
1000.	5000.	6.3054380E 00	7.8874908E-04	-3.4908668E-07	6.8302182E-11	-4.9176506E-15	-1.1913095E 04	-3.5344914E 00
300.	1000.	3.5481932E 00	1.1490821E-02	-1.6741809E-05	1.1703637E-08	-3.1923586E-12	-1.1313991E 04	9.9245853E 00
B1CL3(G)		300.00	5000.00					
1000.	5000.	8.6203460E 00	1.5588465E-03	-6.8620129E-07	1.3355931E-10	-9.5694464E-15	-5.1759400E 04	-1.5290532E 01
300.	1000.	3.1217850E 00	2.2849076E-02	-3.3214510E-05	2.3162470E-08	-6.3018435E-12	-5.0561958E 04	1.1562869E 01
B1F1(G)		300.00	5000.00					
1000.	5000.	3.5528910E 00	1.0662656E-03	-4.4232374E-07	8.4706187E-11	-5.9999521E-15	-2.5138324E 04	3.3860235E 00
300.	1000.	3.5588682E 00	-1.6286373E-03	7.6368278E-06	-8.1504041E-09	2.8388860E-12	-2.5000100E 04	4.0338770E 00
B1F2(G)		300.00	5000.00					
1000.	5000.	5.4047657E 00	1.7569443E-03	-7.6134143E-07	1.4666216E-10	-1.0433260E-14	-6.9724693E 04	-2.0050351E 00
300.	1000.	3.0590521E 00	8.1452471E-03	-6.5334231E-06	1.6970858E-09	1.6863576E-13	-6.9072524E 04	1.0134743E 01
B1F3(G)		300.00	5000.00					
1000.	5000.	6.9712009E 00	3.3291452E-03	-1.4398589E-06	2.7687134E-10	-1.9663726E-14	-1.3844161E 05	-1.0937645E 01
300.	1000.	2.1119086E 00	1.7689399E-02	-1.6876008E-05	7.1126112E-09	-9.2021652E-13	-1.3714589E 05	1.3933536E 01
B1F1CL1(G)		300.00	5000.00					
1000.	5000.	5.9487502E 00	1.1769309E-03	-5.1543517E-07	1.0002224E-10	-7.1535146E-15	-4.1101805E 04	-2.4634651E 00
300.	1000.	3.1915115E 00	1.0620289E-02	-1.3019321E-05	7.6564412E-09	-1.7458071E-12	-4.0439658E 04	1.1307306E 01

B1H1(G)		300.00	5000.00					
1000.	5000.	2.8550687E 00	1.6528384E-03	-6.2466534E-07	1.1285332E-10	-7.6610410E-15	5.5716400E 04	3.9854563E 00
300.	1000.	3.7258740E 00	-1.5968308E-03	3.4172109E-06	-1.6979088E-09	1.4008889E-13	5.5546278E 04	-2.3447266E-01
B1H3(G)		300.00	5000.00					
1000.	5000.	1.9286212E 00	7.5249258E-03	-2.9150822E-06	5.1922764E-10	-3.4891596E-14	8.6871002E 03	9.5682689E 00
300.	1000.	4.0347166E 00	-1.1420593E-03	9.2131971E-06	-6.2604053E-09	1.1773524E-12	8.3241972E 03	-4.2045995E-01
B1N1(G)		300.00	5000.00					
1000.	5000.	3.4469541E 00	1.1674645E-03	-4.7953649E-07	9.0431634E-11	-6.2510633E-15	7.4653488E 04	5.4012515E 00
300.	1000.	3.6749186E 00	-2.2994576E-03	8.4689361E-06	-8.4358062E-09	2.8104731E-12	7.4744375E 04	4.9571132E 00
B1N1(S)		300.00	5000.00					
1000.	5000.	4.0615435E 00	1.7180004E-03	-4.9911199E-07	7.8802658E-11	-5.1372788E-15	-3.2145048E 04	-2.2949093E 01
300.	1000.	-1.1073212E 00	1.6570514E-02	-1.9929047E-05	1.4457119E-08	-4.6371698E-12	-3.0593968E 04	3.9838480E 00
B1O1(G)		300.00	5000.00					
1000.	5000.	3.1114124E 00	1.4660647E-03	-6.0059983E-07	1.1001849E-10	-7.0368629E-15	1.8777191E 03	6.2718598E 00
300.	1000.	3.8411771E 00	-2.8815072E-03	7.7170457E-06	-6.4599236E-09	1.8630677E-12	1.8176566E 03	3.1420279E 00
B1O2(G)		300.00	5000.00					
1000.	5000.	5.6595095E 00	2.0458232E-03	-8.9191322E-07	1.7255128E-10	-1.2314027E-14	-4.4594729E 04	-5.2120875E 00
300.	1000.	2.0440369E 00	1.3046666E-02	-1.3055148E-05	5.6761323E-09	-7.3803048E-13	-4.3656018E 04	1.3190390E 01
B2O2(G)		300.00	5000.00					
1000.	5000.	6.7782064E 00	3.9286353E-03	-1.6590453E-06	3.1432647E-10	-2.2109823E-14	-5.8580478E 04	-1.1457691E 01
300.	1000.	2.6671177E 00	1.9600173E-02	-2.6766238E-05	1.9821426E-08	-5.9824688E-12	-5.7620798E 04	8.8104848E 00
B2O3(G)		300.00	5000.00					
1000.	5000.	6.6342182E 00	6.7755173E-03	-2.8737012E-06	5.4567159E-10	-3.8424386E-14	-1.0848269E 05	-8.3426297E 00
300.	1000.	1.8024791E 00	1.7474524E-02	-8.2523247E-06	-2.0803348E-09	2.0989392E-12	-1.0697856E 05	1.7365142E 01
B2O3(L)		300.00	3500.00					
1000.	5000.	1.5322605E 01	0.	0.	0.	0.	-1.5740266E 05	-8.1439342E 01
300.	1000.	3.6805218E 01	-2.6489662E-01	7.8993534E-04	-8.[illegible]799183E-07	3.4152643E-10	-1.5604006E 05	-1.4928169E 02
B1O1CL1(G)		300.00	5000.00					
1000.	5000.	5.5031930E 00	2.0969014E-03	-8.8218191E-07	1.6665947E-10	-1.1696264E-14	-4.4610112E 04	-3.9025829E 00
300.	1000.	2.5880260E 00	1.4169692E-02	-2.1332608E-05	1.6446286E-08	-4.9985221E-12	-4.3987074E 04	1.0207262E 01
B3O3CL3(G)		300.00	5000.00					
1000.	5000.	1.9802290E 01	5.8745664E-03	-2.5894155E-06	5.0483645E-10	-3.6233293E-14	-2.0936983E 05	-7.3963120E 01
300.	1000.	-3.3878045E-02	8.2746198E-02	-1.2020781E-04	8.3891398E-08	-2.2839870E-11	-2.0504926E 05	2.2903226E 01
B1O1F1(G)		300.00	5000.00					
1000.	5000.	5.0297714E 00	2.5735312E-03	-1.0773675E-06	2.0287789E-10	-1.4206619E-14	-7.3224108E 04	-2.8029988E 00
300.	1000.	2.2253179E 00	1.3012379E-02	-1.7034903E-05	1.1880141E-08	-3.3683309E-12	-7.2568392E 04	1.1055508E 01
B3O3F3(G)		300.00	5000.00					
1000.	5000.	1.8801236E 01	7.0103613E-03	-3.0941469E-06	6.0416288E-10	-4.3427652E-14	-2.9227943E 05	-7.1419556E 01
300.	1000.	-1.4024932E 00	8.0443553E-02	-1.0730304E-04	6.8653568E-08	-1.7113413E-11	-2.8765436E 05	2.8398464E 01
B1S1(G)		300.00	5000.00					
1000.	5000.	3.6003577E 00	1.2278056E-03	-6.5868559E-07	1.6060992E-10	-1.2578712E-14	3.8031894E 04	4.9812773E 00
300.	1000.	3.2283229E 00	6.1853701E-04	3.6449422E-06	-5.2558461E-09	2.0815538E-12	3.8209308E 04	7.2906102E 00
BE1(G)		300.00	5000.00					
1000.	5000.	2.3978915E 00	2.0449278E-04	-1.2906023E-07	2.7413253E-11	-7.7685397E-16	3.8490518E 04	2.6893508E 00
300.	1000.	2.4945010E 00	4.1386213E-05	-1.0781513E-07	1.1661783E-10	-4.4729455E-14	3.8454869E 04	2.1557333E 00
BE1(L)		1556.00	5000.00					
1000.	5000.	3.7740406E 00	-0.	-0.	-0.	-0.	-4.5118896E 02	-2.0819144E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
BE1(S)		300.00	1556.00					
1000.	5000.	2.8926324E 00	-5.3075709E-04	7.4508224E-07	3.6530209E-10	-1.9839302E-13	-9.5512609E 02	-1.5490516E 01
300.	1000.	-1.0397013E 00	1.6815433E-02	-2.8775045E-05	2.3342718E-08	-7.0695416E-12	-2.2596996E 02	3.1456032E 00
BE1CL1(G)		300.00	5000.00					
1000.	5000.	4.0942748E 00	5.0067207E-04	-1.9518744E-07	3.6432020E-11	-2.3966847E-15	1.7294492E 04	2.4707799E 00
300.	1000.	2.7178220E 00	5.2788145E-03	-6.5064710E-06	3.7476141E-09	-8.0398524E-13	1.7618157E 04	9.3198141E 00
BE1CL2(G)		300.00	5000.00					
1000.	5000.	6.4539849E 00	1.1861923E-03	-5.2491041E-07	1.0273231E-10	-7.3994416E-15	-4.5684370E 04	-8.4512879E 00
300.	1000.	2.4650300E 00	1.6818399E-02	-2.4729612E-05	1.7461162E-08	-4.8043815E-12	-4.4823496E 04	1.0986682E 01
BE1CL2(L)		678.00	5000.00					
1000.	5000.	1.1070519E 01	-0.	-0.	-0.	-0.	-6.1900929E 04	-5.1770676E 01
300.	1000.	1.1070519E 01	-0.	-0.	-0.	-0.	-6.1900929E 04	-5.1770676E 01
BE1CL2(S)		300.00	678.00					
1000.	5000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
300.	1000.	5.4849391E 00	7.4977606E-03	-0.	-0.	-0.	-6.1346824E 04	-2.2667512E 01
BE1F1(G)		300.00	5000.00					
1000.	5000.	3.7000317E 00	9.1285560E-04	-3.7407805E-07	7.0937271E-11	-4.9326462E-15	6.8706450E 02	3.2036670E 00
300.	1000.	3.3508932E 00	-2.5760447E-04	5.3169342E-06	-6.5525393E-09	2.4471316E-12	8.8988562E 02	5.5351947E 00
BE1F2(G)		300.00	5000.00					
1000.	5000.	5.3886642E 00	2.3309245E-03	-1.0113536E-06	1.9495829E-10	-1.3874162E-14	-9.3965418E 04	-5.6529548E 00
300.	1000.	1.3850116E 00	1.4634404E-02	-1.4883871E-05	6.7312589E-09	-9.7748477E-13	-9.2930686E 04	1.4698212E 01
BE1F2(L)		1070.00	5000.00					
1000.	5000.	1.2076930E 01	-0.	-0.	-0.	-0.	-1.2457152E 05	-6.3559840E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
BE1F2(S)		300.00	1070.00					
1000.	5000.	8.2726971E 00	5.1025028E-04	-0.	-0.	-0.	-1.2381218E 05	-4.0392709E 01
300.	1000.	8.2726971E 00	5.1025028E-04	-0.	-0.	-0.	-1.2381218E 05	-4.0392709E 01
BE1F1CL1(G)		300.00	5000.00					
1000.	5000.	5.9472074E 00	1.7304756E-03	-7.5551323E-07	1.4628105E-10	-1.0444067E-14	-7.0010254E 04	-6.5405302E 00
300.	1000.	1.6705781E 00	1.7255147E-02	-2.3000996E-05	1.4987230E-08	-3.8539546E-12	-6.9022337E 04	1.4613342E 01
BE1H1(G)		300.00	5000.00					
1000.	5000.	3.0170590E 00	1.5728187E-03	-6.1395392E-07	1.1380482E-10	-7.8746509E-15	3.8327846E 04	3.6069494E 00
300.	1000.	3.8113634E 00	-2.4852219E-03	6.3094992E-06	-4.7649985E-09	1.2112125E-12	3.8230628E 04	3.7899569E-02
BE1O1(G)		300.00	5000.00					
1000.	5000.	4.1807162E 00	-2.4834712E-04	3.5022984E-07	-5.5095477E-11	1.6058349E-15	1.3916785E 04	-3.6730129E-01
300.	1000.	3.6652305E 00	-2.2914647E-03	8.7253562E-06	-8.9055942E-09	3.0356028E-12	1.4267956E 04	3.2407899E 00
BE1O1(L)		2843.00	5000.00					
1000.	5000.	7.2964787E 00	0.	0.	0.	0.	-6.8666976E 04	-4.0840683E 01
300.	1000.	0.	0.	0.	0.	0.	0.	0.
BE1O1(S)		300.00	2843.00					
1000.	5000.	4.1238290E 00	2.6898164E-03	-1.0772104E-06	2.0353250E-10	-1.4413285E-14	-7.3636946E 04	-2.3246285E 01
300.	1000.	-3.5322081E 00	3.5547229E-02	-5.6822096E-05	4.3746057E-08	-1.3013435E-11	-7.2113816E 04	1.3390352E 01

BE1O2H2(G)		300.00	5000.00					
1000.	5000.	4.1830391E 00	8.4982247E-03	-3.2651229E-06	5.8056899E-10	-3.9061373E-14	-8.3624839E 04	-1.2865596E-01
300.	1000.	2.4483689E 00	7.5396683E-03	9.5058239E-06	-1.5633564E-08	6.0973542E-12	-8.2841623E 04	1.0297711E 01
BE2O2(G)		300.00	5000.00					
1000.	5000.	7.2656515E 00	3.0436593E-03	-1.3278244E-06	2.5695786E-10	-1.8339204E-14	-5.5252811E 04	-1.2939644E 01
300.	1000.	2.2982095E 00	1.6953025E-02	-1.4266072E-05	3.8338247E-09	4.0111862E-13	-5.3905411E 04	1.2636834E 01
BE3O3(G)		300.00	5000.00					
1000.	5000.	1.0223629E 01	6.4242786E-03	-2.7986060E-06	5.4071499E-10	-3.8530851E-14	-1.3260649E 05	-2.9645351E 01
300.	1000.	-1.3603821E 00	4.0799953E-02	-3.8954026E-05	1.5142194E-08	-1.2762531E-12	-1.2956134E 05	2.9518470E 01
BE4O4(G)		300.00	5000.00					
1000.	5000.	1.4164162E 01	8.7368891E-03	-3.8154943E-06	7.3888569E-10	-5.2761944E-14	-1.9522886E 05	-5.0967451E 01
300.	1000.	-2.4980528E 00	6.0319132E-02	-6.2442512E-05	2.8686049E-08	-4.2929379E-12	-1.9095419E 05	3.3606638E 01
C1(G)		300.00	5000.00					
1000.	5000.	2.5793248E 00	-1.4336257E-04	7.2089675E-08	-7.3755078E-12	1.0107793E-17	8.5425628E 04	4.3223635E 00
300.	1000.	2.5407293E 00	-2.1936478E-04	4.6748747E-07	-4.4444733E-10	1.5628193E-13	8.5448440E 04	4.5738974E 00
C1(S)		300.00	4000.00					
1000.	5000.	1.3522089E 00	1.8787960E-03	-7.8222605E-07	1.5535768E-10	-1.1814441E-14	-6.4583539E 02	-7.9293986E 00
300.	1000.	-6.4250569E-01	6.8262474E-03	-4.2255719E-06	1.5222307E-10	4.8192939E-13	-7.5029564E 01	2.5014319E 00
C2(G)		300.00	5000.00					
1000.	5000.	4.0441743E 00	1.7207013E-04	1.5709175E-07	-5.4885609E-11	4.8258945E-15	9.9610196E 04	1.2880976E 00
300.	1000.	7.5038971E 00	-1.0609454E-02	9.9776828E-06	-7.5630531E-10	-1.7925449E-12	9.8802536E 04	-1.6056443E 01
C3(G)		300.00	5000.00					
1000.	5000.	4.7124744E 00	2.9026521E-03	-1.2142448E-06	2.2847047E-10	-1.5986400E-14	9.3752700E 04	-2.5304385E 00
300.	1000.	2.6325874E 00	9.4185729E-03	-9.5932409E-06	5.5795525E-09	-1.4241068E-12	9.4311478E 04	8.0788261E 00
C1CL1(G)		300.00	5000.00					
1000.	5000.	4.1002973E 00	4.9047672E-04	-1.9710270E-07	3.8183019E-11	-2.7164997E-15	6.0283800E 04	3.3198825E 00
300.	1000.	3.1228619E 00	3.3329302E-03	-2.9580437E-06	8.6082075E-10	7.0568687E-14	6.0540006E 04	8.3172500E 00
C1CL4(G)		300.00	5000.00					
1000.	5000.	1.1506170E 01	1.7129154E-03	-7.6324114E-07	1.5007068E-10	-1.0844894E-14	-1.6652707E 04	-2.9550476E 01
300.	1000.	3.3645211E 00	3.5599740E-02	-5.6167723E-05	4.1742284E-08	-1.1943756E-11	-1.4997781E 04	9.6246173E 00
C1F1(G)		300.00	5000.00					
1000.	5000.	3.6640409E 00	9.5846955E-04	-3.9586490E-07	7.6136251E-11	-5.4116391E-15	3.6376130E 04	4.2853585E 00
300.	1000.	3.5867220E 00	-1.5380358E-03	7.7687077E-06	-8.6182187E-09	3.0982182E-12	3.6533051E 04	5.3559095E 00
C1F2(G)		300.00	5000.00					
1000.	5000.	5.0791144E 00	2.1918640E-03	-9.2233106E-07	1.7815640E-10	-1.2704054E-14	-1.6621332E 04	-1.2059364E 00
300.	1000.	2.9608436E 00	5.9032634E-03	3.1072007E-07	-5.2530054E-09	2.5922796E-12	-1.5932984E 04	1.0257778E 01
C1F3(G)		300.00	5000.00					
1000.	5000.	6.9700395E 00	3.7894531E-03	-1.4396634E-06	2.7674547E-10	-1.9648272E-14	-6.2712536E 04	-1.0311075E 01
300.	1000.	1.9510288E 00	1.8725713E-02	-1.7690562E-05	7.6601723E-09	-1.0694265E-12	-6.1380591E 04	1.5349513E 01
C1F4(G)		300.00	5000.00					
1000.	5000.	9.0219456E 00	4.8141869E-03	-1.9233018E-06	3.7153520E-10	-2.6475250E-14	-1.1274889E 05	-2.2627487E 01
300.	1000.	4.2603580E-01	3.2316566E-02	-3.5029545E-05	1.7874827E-08	-3.3299949E-12	-1.1058388E 05	2.0793144E 01
C1H1(G)		300.00	5000.00					
1000.	5000.	1.9575667E 00	3.3180103E-03	-1.4731439E-06	2.9373595E-10	-2.1308003E-14	7.1060030E 04	1.0225158E 01
300.	1000.	3.5360200E 00	1.5295029E-04	-1.9992575E-06	4.6461050E-09	-2.2609579E-12	7.0599316E 04	1.8588287E 00
C1H2(G)		300.00	5000.00					
1000.	5000.	2.2080673E 00	4.7528351E-03	-1.7927054E-06	3.1323663E-10	-2.0754448E-14	3.3843045E 04	7.8268502E 00
300.	1000.	3.5211754E 00	-2.2791581E-03	1.1759517E-05	-1.1104759E-08	3.5639032E-12	3.3666093E 04	1.9219359E 00
C1H3(G)		300.00	5000.00					
1000.	5000.	2.7755430E 00	6.3035762E-03	-2.3230844E-06	3.9853794E-10	-2.6026064E-14	1.5793539E 04	5.8334007E 00
300.	1000.	3.3813474E 00	4.4056034E-03	-1.5919182E-07	-7.5866050E-10	2.5944831E-13	1.5647628E 04	2.7790427E 00
C1H4(G)		300.00	5000.00					
1000.	5000.	1.1795744E 00	1.0950594E-02	-4.0622131E-06	7.1370281E-10	-4.7490353E-14	-9.8556627E 03	1.2505934E 01
300.	1000.	4.2497678E 00	-6.9126562E-03	3.1602134E-05	-2.9715432E-08	9.5103580E-12	-1.0186632E 04	-9.1754991E-01
C2H2(G) C_2H_2		300.00	5000.00					
1000.	5000.	4.4778953E 00	5.3099467E-03	-1.8636017E-06	3.1648036E-10	-2.0523151E-14	2.5643639E 04	-3.0441023E 00
300.	1000.	8.0198216E-01	2.3378358E-02	-3.5299965E-05	2.7684824E-08	-8.3450065E-12	2.6253611E 04	1.3956314E 01
C2H4(G) C_2H_4		300.00	5000.00					
1000.	5000.	3.4537560E 00	1.1687057E-02	-4.5351384E-06	8.0987972E-10	-5.4572967E-14	4.4721772E 03	2.7323118E 00
300.	1000.	1.0971215E 00	1.4081757E-02	2.1916922E-06	-1.1049911E-08	5.0403237E-12	5.3351537E 03	1.5932790E 01
C1N1(G)		300.00	5000.00					
1000.	5000.	3.6068209E 00	3.3196336E-04	1.0279205E-07	-1.7235337E-11	-2.9277077E-16	4.7308710E 04	3.5270902E 00
300.	1000.	3.8528145E 00	-2.7632042E-03	6.8570434E-06	-5.4131979E-09	1.4905933E-12	4.7409697E 04	2.9718018E 00
C2N2(G)		300.00	5000.00					
1000.	5000.	6.5024264E 00	4.0532184E-03	-1.6639966E-06	3.0947405E-10	-2.1482992E-14	3.4904749E 04	-9.4419093E 00
300.	1000.	3.4026925E 00	1.7756299E-02	-2.6860559E-05	2.1968412E-08	-7.0872074E-12	3.5550207E 04	5.4122791E 00
C1O1(G)		300.00	5000.00					
1000.	5000.	2.9537179E 00	1.5476609E-03	-6.1603844E-07	1.1272797E-10	-7.7208967E-15	-1.4232807E 04	6.5172790E 00
300.	1000.	3.7929971E 00	-2.2156370E-03	5.1939122E-06	-3.6035264E-09	8.2262203E-13	-1.4364082E 04	2.6092518E 00
C1O2(G)		300.00	5000.00					
1000.	5000.	4.4008955E 00	3.2163852E-03	-1.3134666E-06	2.4548216E-10	-1.7094645E-14	-4.8940097E 04	-6.6437717E-01
300.	1000.	2.1974487E 00	1.0163064E-02	-1.0164894E-05	5.7246714E-09	-1.3880886E-12	-4.8355113E 04	1.0551881E 01
C1O1CL2(G)		300.00	5000.00					
1000.	5000.	7.6818485E 00	2.5120332E-03	-1.0776482E-06	2.0619275E-10	-1.4596992E-14	-2.9469426E 04	-1.0945890E 01
300.	1000.	2.4834310E 00	2.3088765E-02	-3.4041696E-05	2.5093821E-08	-7.3164953E-12	-2.8332887E 04	1.4398394E 01
C1O1CL1F1(G)		300.00	5000.00					
1000.	5000.	7.1152340E 00	3.1317698E-03	-1.3453946E-06	2.5771199E-10	-1.8261203E-14	-5.5225670E 04	-8.8047161E 00
300.	1000.	1.8378727E 00	2.1766280E-02	-2.7393349E-05	1.7467802E-08	-4.4775274E-12	-5.3963572E 04	1.7477611E 01
C1O1F2(G)		300.00	5000.00					
1000.	5000.	6.4817495E 00	3.8193318E-03	-1.6418840E-06	3.1482319E-10	-2.2332894E-14	-8.0953679E 04	-7.7207056E 00
300.	1000.	1.4280294E 00	1.9250230E-02	-1.9270666E-05	9.0935910E-09	-1.5494981E-12	-7.9628408E 04	1.8028182E 01
C1O1S1(G)		300.00	5000.00					
1000.	5000.	5.1879121E 00	2.5067857E-03	-1.0247238E-06	1.9383567E-10	-1.3621126E-14	-1.8321013E 04	-2.8104775E 00
300.	1000.	2.0900133E 00	1.4597870E-02	-2.0419577E-05	1.5010523E-08	-4.4266421E-12	-1.7624273E 04	1.2361751E 01
C1S1(G)		300.00	5000.00					
1000.	5000.	3.6767641E 00	9.2651925E-04	-3.8859937E-07	7.4368526E-11	-5.2463347E-15	2.6292259E 04	3.9148053E 00
300.	1000.	3.3962380E 00	-5.7451495E-04	5.9067212E-06	-7.0446431E-09	2.6000062E-12	2.6483564E 04	5.9276761E 00
C1S2(G)		300.00	5000.00					
1000.	5000.	5.9369726E 00	1.8016390E-03	-7.3714320E-07	1.4104199E-10	-9.9941705E-15	1.1814715E 04	-6.1474592E 00
300.	1000.	2.8623344E 00	1.2953197E-02	-1.7126738E-05	1.1649384E-08	-3.2056632E-12	1.2538820E 04	9.0974305E 00

CA1(G)		300.00	5000.00					
1000.	5000.	1.6749540E 00	1.8558886E-03	-1.4101628E-06	4.1391974E-10	-3.4569433E-14	2.0760477E 04	8.7902632E 00
300.	1000.	2.5044392E 00	-3.3378350E-05	8.6841220E-08	-9.3793153E-11	3.5921133E-14	2.0489455E 04	4.3527623E 00
CL1(G)		300.00	5000.00					
1000.	5000.	2.9657881E 00	-4.3004990E-04	1.6643053E-07	-2.9717571E-11	2.0047255E-15	1.3670965E 04	3.0001737E 00
300.	1000.	1.9842061E 00	3.6198919E-03	-6.0840653E-06	4.2326431E-09	-1.0782205E-12	1.3861529E 04	7.7052771E 00
CL2(G)		300.00	5000.00					
1000.	5000.	4.3120535E 00	2.7351354E-04	-9.2259884E-08	1.7749065E-11	-1.2566223E-15	-1.3447369E 03	2.0545109E 00
300.	1000.	2.9388173E 00	6.2636200E-03	-1.0320071E-05	7.9903872E-09	-2.3629547E-12	-1.0781035E 03	8.5971680E 00
CL1C1N1(G)		300.00	5000.00					
1000.	5000.	5.3603966E 00	2.1838514E-03	-9.0282725E-07	1.6867718E-10	-1.1751590E-14	1.4134474E 04	-3.0060154E 00
300.	1000.	2.9788646E 00	1.2790577E-02	-2.0112266E-05	1.6283242E-08	-5.1420735E-12	1.4613212E 04	8.3540775E 00
CL1F1(G)		300.00	5000.00					
1000.	5000.	4.1495303E 00	4.8298836E-04	-1.7052065E-07	3.2826026E-11	-2.3284128E-15	-8.0973532E 03	2.2586947E 00
300.	1000.	2.7134146E 00	5.7620875E-03	-7.6532634E-06	4.8261343E-09	-1.1558779E-12	-7.7741569E 03	9.3319199E 00
CL1F3(G)		300.00	5000.00					
1000.	5000.	8.9129541E 00	1.2550383E-03	-5.6216105E-07	1.1099172E-10	-8.0475754E-15	-2.2448643E 04	-1.7873577E 01
300.	1000.	1.9837740E 00	3.1211177E-02	-5.1355206E-05	3.9531326E-08	-1.1662299E-11	-2.1090751E 04	1.5205337E 01
CL1O1(G)		300.00	5000.00					
1000.	5000.	4.0852646E 00	4.9908880E-04	-1.9276597E-07	3.5467038E-11	-2.3272475E-15	1.0863357E 04	3.6441914E 00
300.	1000.	2.7097948E 00	5.2540238E-03	-6.5119800E-06	3.8409438E-09	-8.6805562E-13	1.1189541E 04	1.0498211E 01
CL1O2(G)		300.00	5000.00					
1000.	5000.	5.6845585E 00	1.5554443E-03	-6.4426875E-07	1.2495456E-10	-8.9321992E-15	1.0617978E 04	-2.4192053E 00
300.	1000.	2.7120020E 00	1.0556362E-02	-1.0311884E-05	4.1101144E-09	-3.5483798E-13	1.1385505E 04	1.2705468E 01
CL2O1(G)		300.00	5000.00					
1000.	5000.	6.1295246E 00	9.8370521E-04	-4.3316926E-07	8.4340974E-11	-6.0450358E-15	7.0759267E 03	-3.5699167E 00
300.	1000.	2.8367006E 00	1.3274620E-02	-1.8343989E-05	1.2066459E-08	-3.0754364E-12	7.8119147E 03	1.2613908E 01
F1(G)		300.00	5000.00					
1000.	5000.	2.6959312E 00	-2.1447184E-04	9.2868868E-08	-1.7910205E-11	1.2762900E-15	8.7171463E 03	3.8314370E 00
300.	1000.	2.7898969E 00	1.4936162E-04	-1.6455151E-06	2.0348707E-09	-7.7092015E-13	8.6619693E 03	3.1964920E 00
F2(G)		300.00	5000.00					
1000.	5000.	4.0314229E 00	6.1671059E-04	-2.2628668E-07	4.3517814E-11	-3.0857270E-15	-1.3091705E 03	1.0435338E 00
300.	1000.	2.7493810E 00	4.7101738E-03	-5.0359911E-06	2.4217261E-09	-3.8301132E-13	-9.8919251E 02	7.5131989E 00
H1(G)		300.00	5000.00					
1000.	5000.	2.5026549E 00	-5.2597415E-06	3.3319780E-09	-8.3272843E-13	7.1462541E-17	2.5471626E 04	-4.7447219E-01
300.	1000.	2.4948264E 00	3.8845703E-05	-1.0089808E-07	1.0880690E-10	-4.1615102E-14	2.5473072E 04	-4.3851027E-01
H2(G)		300.00	5000.00					
1000.	5000.	3.0798700E 00	5.4216636E-04	3.8487619E-08	-3.4633889E-11	3.6719053E-15	-8.6892051E 02	-1.8472212E 00
300.	1000.	2.8612126E 00	4.0632815E-03	-9.1926019E-06	8.9489950E-09	-3.0513266E-12	-9.6869866E 02	-1.4731534E 00
H1B1O2(G)		300.00	5000.00					
1000.	5000.	4.6528412E 00	4.9420924E-03	-1.9158089E-06	3.4262774E-10	-2.3142282E-14	-7.0084991E 04	4.9686799E-01
300.	1000.	2.7834325E 00	8.5374964E-03	-2.0982812E-06	-2.8829896E-09	1.6595529E-12	-6.9482296E 04	1.0561250E 01
H3B1O3(G)		300.00	5000.00					
1000.	5000.	8.2749906E 00	1.0040200E-02	-3.9174457E-06	7.0308879E-10	-4.7582380E-14	-1.2341623E 05	-1.7777290E 01
300.	1000.	1.0154671E 00	3.3238342E-02	-3.1352477E-05	1.4408543E-08	-2.2566237E-12	-1.2159532E 05	1.8872871E 01
H3B3O6(G)		300.00	5000.00					
1000.	5000.	1.9964743E 01	1.3419223E-02	-5.3345453E-06	9.7213542E-10	-6.6597355E-14	-2.8057384E 05	-7.8677512E 01
300.	1000.	-4.5566096E 00	1.0336231E-01	-1.3249504E-04	8.2303669E-08	-1.9659383E-11	-2.7505153E 05	4.2134826E 01
H1CL1(G)		300.00	5000.00					
1000.	5000.	2.7356497E 00	1.4979644E-03	-5.0699071E-07	8.2790246E-11	-5.1747522E-15	-1.1906174E 04	6.6280129E 00
300.	1000.	3.5127954E 00	1.0648349E-04	-1.0344968E-06	2.2632198E-09	-1.0437634E-12	-1.2149134E 04	2.4477521E 00
H1C1N1(G)		300.00	5000.00					
1000.	5000.	3.6403265E 00	3.4732994E-03	-1.2682652E-06	2.2079754E-10	-1.4559323E-14	1.4426168E 04	2.4445637E 00
300.	1000.	2.1711349E 00	1.0702257E-02	-1.5003573E-05	1.1853276E-08	-3.6714972E-12	1.4682584E 04	9.2688169E 00
H1C1O1(G)		300.00	5000.00					
1000.	5000.	3.2708241E 00	3.5195799E-03	-1.3772859E-06	2.4731356E-10	-1.6727435E-14	-2.7820147E 03	7.3044232E 00
300.	1000.	3.8647056E 00	-5.3708648E-04	6.9034500E-06	-6.6450605E-09	2.0576966E-12	-2.7995993E 03	4.8971867E 00
H1F1(G)		300.00	5000.00					
1000.	5000.	3.0027529E 00	6.9264447E-04	-5.3422875E-08	-1.4891104E-11	2.3158465E-15	-3.3452607E 04	3.7531290E 00
300.	1000.	3.4714781E 00	2.8482667E-04	-8.6756213E-07	1.0442415E-09	-3.0358504E-13	-3.3649646E 04	1.0536081E 00
H2O1(G)		300.00	5000.00					
1000.	5000.	2.6707532E 00	3.0317115E-03	-8.5351570E-07	1.1790853E-10	-6.1973568E-15	-2.9888994E 04	6.8838391E 00
300.	1000.	4.1565016E 00	-1.7244334E-03	5.6982316E-06	-4.5930044E-09	1.4233654E-12	-3.0288770E 04	-6.8616246E-01
H1S1(G)		300.00	5000.00					
1000.	5000.	2.9739815E 00	1.3871555E-03	-4.8940351E-07	8.3643125E-11	-5.4502127E-15	1.7393974E 04	6.4256706E 00
300.	1000.	4.2680376E 00	-1.3506075E-03	-6.4336118E-07	3.6149570E-09	-1.9391003E-12	1.7024020E 04	-3.9230257E-01
H2S1(G)		300.00	5000.00					
1000.	5000.	2.7657149E 00	4.0131914E-03	-1.5044898E-06	2.6807998E-10	-1.7967681E-14	-3.3859808E 03	7.9327186E 00
300.	1000.	3.9163074E 00	-3.5138671E-04	4.2191312E-06	-2.7453665E-09	4.8584365E-13	-3.6095585E 03	2.3660042E 00
HE1(G)		300.00	5000.00					
1000.	5000.	2.5002058E 00	-3.4269657E-07	1.9577345E-10	-4.6329409E-14	3.8726676E-18	-8.9092124E-02	9.1429628E-01
300.	1000.	2.5001399E 00	-1.4456334E-06	5.0497579E-09	-6.9020475E-12	3.1744021E-15	-9.9023618E-03	9.1492015E-01
K1(G)		300.00	5000.00					
1000.	5000.	2.2547143E 00	5.7663084E-04	-4.6267401E-07	1.4248137E-10	-1.1230833E-14	1.0111123E 04	6.3316717E 00
300.	1000.	2.4875524E 00	9.3590544E-05	-2.4349660E-07	2.6299618E-10	-1.0072091E-13	1.0034515E 04	5.0789355E 00
LI1(G)		300.00	5000.00					
1000.	5000.	2.4139909E 00	2.1594723E-04	-1.8433641E-07	5.9041104E-11	-4.6253608E-15	1.8624119E 04	2.8858270E 00
300.	1000.	2.4988538E 00	7.9504246E-06	-1.8505802E-08	1.7547754E-11	-5.8286802E-15	1.8598592E 04	2.4388285E 00
LI1(L)		453.70	2500.00					
1000.	5000.	3.4942584E 00	-2.7676298E-05	-0.	-0.	-0.	-6.9517827E 02	-1.5680612E 01
300.	1000.	5.2552318E 00	-5.6671376E-03	5.4991596E-06	-9.5345869E-10	-6.7059797E-13	-1.0965420E 03	-2.4468648E 01
LI1(S)		300.00	453.70					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	2.8012940E 00	1.1861188E-04	-3.6540493E-06	2.0437288E-08	-1.0229216E-11	-8.4371812E 02	-1.2498461E 01
LI2(G)		300.00	5000.00					
1000.	5000.	4.4199526E 00	2.5890334E-04	-4.1884761E-08	8.2816832E-12	-6.0073758E-16	2.4045151E 04	-1.6359295E 00
300.	1000.	3.6167674E 00	4.0128034E-03	-6.8310298E-06	5.5504691E-09	-1.7040589E-12	2.4189654E 04	2.1315175E 00
LI1CL1(G)		300.00	5000.00					
1000.	5000.	4.2503226E 00	3.6496125E-04	-1.2808936E-07	2.5216315E-11	-1.8243732E-15	-2.4095699E 04	1.1348996E 00
300.	1000.	2.7911617E 00	6.4519652E-03	-1.0066518E-05	7.4516559E-09	-2.1176767E-12	-2.3800670E 04	8.1501199E 00

LI1CL1(L)		880.00	5000.00					
1000.	5000.	7.7745237E 00	-0.	-0.	-0.	-0.	-4.9762536E 04	-3.6766096E 01
300.	1000.	7.7745237E 00	-0.	-0.	-0.	-0.	-4.9762536E 04	-3.6766096E 01
LI1CL1(S)		300.00	880.00					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	3.8578623E 00	1.0403508E-02	-1.7735170E-05	1.7820003E-08	-6.7139562E-12	-5.0651157E 04	-1.8237936E 01
LI2CL2(G)		300.00	5000.00					
1000.	5000.	9.4955231E 00	5.8171912E-04	-2.5889458E-07	5.0690504E-11	-3.6435654E-15	-7.5393890E 04	-1.9873584E 01
300.	1000.	4.4900863E 00	2.3990713E-02	-4.2719507E-05	3.4871351E-08	-1.0767253E-11	-7.4491856E 04	3.6080745E 00
LI1F1(G)		300.00	5000.00					
1000.	5000.	4.0395917E 00	5.8209706E-04	-2.2261733E-07	4.2814205E-11	-3.0356123E-15	-4.1213860E 04	6.8177847E-01
300.	1000.	2.7393082E 00	4.8069812E-03	-5.3497046E-06	2.7428441E-09	-5.0057916E-13	-4.0892489E 04	7.2268538E 00
LI1F1(L)		1121.00	5000.00					
1000.	5000.	7.7040750E 00	-0.	-0.	-0.	-0.	-7.3712704E 04	-3.8719372E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
LI1F1(S)		300.00	1121.00					
1000.	5000.	5.1340557E 00	3.7670728E-03	-5.4430681E-06	4.5584666E-09	-8.5384268E-13	-7.5395926E 04	-2.6184493E 01
300.	1000.	8.0628070E-01	2.3602744E-02	-4.0828340E-05	3.3413011E-08	-9.8310149E-12	-7.4609098E 04	-5.8062076E 00
LI2F2(G)		300.00	5000.00					
1000.	5000.	9.1949698E 00	9.3004194E-04	-4.1582671E-07	8.1873703E-11	-5.9187496E-15	-1.1499626E 05	-2.1514750E 01
300.	1000.	2.6450457E 00	3.0557012E-02	-5.2666426E-05	4.1967247E-08	-1.2717744E-11	-1.1377194E 05	9.4450153E 00
LI3F3(G)		300.00	5000.00					
1000.	5000.	1.2888686E 01	3.5230060E-03	-1.5545971E-06	3.0329660E-10	-2.1777982E-14	-1.7832249E 05	-4.0009658E 01
300.	1000.	1.5326555E 00	4.5414791E-02	-6.1760529E-05	3.9967174E-08	-1.0015482E-11	-1.7576094E 05	1.5923332E 01
LI1H1(G)		300.00	5000.00					
1000.	5000.	3.5617370E 00	1.1259789E-03	-4.3721607E-07	8.3615353E-11	-5.9148090E-15	1.5741115E 04	-2.4211284E-01
300.	1000.	3.5048021E 00	-1.2466224E-03	6.9927550E-06	-7.5558750E-09	2.6331419E-12	1.5889755E 04	6.9552820E-01
LI1O1(G)		300.00	5000.00					
1000.	5000.	3.9094136E 00	7.1351566E-04	-2.8477513E-07	5.4871902E-11	-3.9001186E-15	5.7645304E 03	2.1331190E 00
300.	1000.	2.9569606E 00	2.7495441E-03	-7.1016591E-07	-1.5182148E-09	9.1100243E-13	6.0510574E 03	7.1847356E 00
LI2O1(G)		300.00	5000.00					
1000.	5000.	5.5053346E 00	1.6753178E-03	-7.3444785E-07	1.4265854E-10	-1.0211945E-14	-2.1032422E 04	-4.2061218E 00
300.	1000.	2.3130146E 00	1.0884968E-02	-9.6808751E-06	2.9020082E-09	1.5953552E-13	-2.0186572E 04	1.2146986E 01
LI2O1(L)		1700.00	5000.00					
1000.	5000.	1.2076930E 01	-0.	-0.	-0.	-0.	-7.0648682E 04	-6.4640360E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
LI2O1(S)		300.00	1700.00					
1000.	5000.	3.8995906E 00	1.1789318E-02	-8.2228955E-06	3.4773552E-09	-5.5080702E-13	-7.3198682E 04	-2.0745283E 01
300.	1000.	-2.5550786E 00	5.2344640E-02	-9.6543893E-05	8.5443840E-08	-2.8296961E-11	-7.2523735E 04	7.0615398E 00
LI1O1H1(G)		300.00	5000.00					
1000.	5000.	4.1181831E 00	2.3526905E-03	-8.2767084E-07	1.3743995E-10	-8.7691556E-15	-3.0195411E 04	2.1508534E 00
300.	1000.	3.0906573E 00	4.1274403E-03	6.9269641E-07	-4.2945684E-09	2.1556489E-12	-2.9886931E 04	7.6500483E 00
LI1O1H1(L)		744.30	5000.00					
1000.	5000.	1.0436480E 01	-0.	-0.	-0.	-0.	-6.0393496E 04	-5.3644760E 01
300.	1000.	1.0436480E 01	-0.	-0.	-0.	-0.	-6.0393496E 04	-5.3644760E 01
LI1O1H1(S)		300.00	744.30					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	-2.5965216E 00	5.3071043E-02	-1.1312408E-04	1.2020097E-07	-4.8500607E-11	-2.9359207E 04	8.1817051E 00
LI2O2H2(G)		300.00	5000.00					
1000.	5000.	9.4722433E 00	5.5785561E-03	-2.0423512E-06	3.5052228E-10	-2.2972242E-14	-9.2726531E 04	-2.3519482E 01
300.	1000.	1.5953202E 00	3.5601754E-02	-4.5943003E-05	2.9291286E-08	-7.2093621E-12	-9.1025571E 04	1.4969178E 01
MG1(G)		300.00	5000.00					
1000.	5000.	2.4043590E 00	1.9005770E-04	-1.1793682E-07	2.3792231E-11	-3.3893521E-16	1.7202796E 04	4.1436162E 00
300.	1000.	2.4896392E 00	7.7811114E-05	-2.0215519E-07	2.1803364E-10	-8.3395625E-14	1.7169763E 04	3.6648936E 00
MG1(L)		923.00	2500.00					
1000.	5000.	2.3968576E 00	1.9607149E-03	-5.9072332E-07	2.3152117E-10	-3.3102729E-14	2.9941793E 02	-9.0899473E 00
300.	1000.	-1.2076232E 00	1.2591523E-02	-1.0151878E-05	1.8860340E-09	8.4721272E-13	1.1858554E 03	9.1871104E 00
MG1(S)		300.00	923.00					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	2.6724626E 00	1.0280450E-03	-1.5966099E-07	1.4113027E-09	-8.6630548E-13	-8.4346544E 02	-1.1612203E 01
MG1CL1(G)		300.00	5000.00					
1000.	5000.	4.3693863E 00	2.0291060E-04	-6.1061697E-08	1.0431818E-11	-5.2222300E-16	-5.8761307E 02	3.0160849E 00
300.	1000.	3.2096883E 00	5.4943849E-03	-9.4731671E-06	7.6160759E-09	-2.3258383E-12	-3.7263176E 02	8.4876869E 00
MG1CL2(G)		300.00	5000.00					
1000.	5000.	7.1103608E 00	4.5064700E-04	-2.0163150E-07	3.9715346E-11	-2.8715039E-15	-5.2961128E 04	-9.9360510E 00
300.	1000.	3.8279892E 00	1.5386366E-02	-2.6656943E-05	2.1304965E-08	-6.4661607E-12	-5.2351835E 04	5.5571101E 00
MG1CL2(L)		987.00	5000.00					
1000.	5000.	1.1120840E 01	-0.	-0.	-0.	-0.	-7.6361421E 04	-4.9333501E 01
300.	1000.	1.1120840E 01	-0.	-0.	-0.	-0.	-7.6361421E 04	-4.9333501E 01
MG1CL2(S)		300.00	987.00					
1000.	5000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
300.	1000.	1.5726281E 00	3.6191610E-02	-5.4077678E-05	2.7099282E-08	-0.	-7.8844972E 04	-6.8179675E 00
MG1F1(G)		300.00	5000.00					
1000.	5000.	4.2063912E 00	3.7247087E-04	-1.3734467E-07	2.4894861E-11	-1.5516431E-15	-1.1519246E 04	2.3507615E 00
300.	1000.	2.7293920E 00	6.1504978E-03	-8.9508238E-06	6.1671103E-09	-1.6313164E-12	-1.1203035E 04	9.5422596E 00
MG1F2(G)		300.00	5000.00					
1000.	5000.	6.7119472E 00	9.0253334E-04	-4.0111766E-07	7.8632441E-11	-5.6653499E-15	-9.2190411E 04	-1.0803550E 01
300.	1000.	1.8137078E 00	2.1879751E-02	-3.5656281E-05	2.7220275E-08	-7.9711261E-12	-9.1221380E 04	1.2626802E 01
MG1F2(L)		1536.00	5000.00					
1000.	5000.	1.1404648E 01	-0.	-0.	-0.	-0.	-1.3169142E 05	-5.7366906E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
MG1F2(S)		300.00	1536.00					
1000.	5000.	8.1014253E 00	-8.6389773E-06	3.9829583E-06	-3.2468864E-09	8.4023911E-13	-1.3536571E 05	-3.9640827E 01
300.	1000.	1.3284756E 00	3.4723463E-02	-6.2150671E-05	5.2416429E-08	-1.6648607E-11	-1.3433233E 05	-8.7024649E 00
MG1F1CL1(G)		300.00	5000.00					
1000.	5000.	6.9151697E 00	6.7163191E-04	-2.9859845E-07	5.8489748E-11	-4.2088436E-15	-7.2583497E 04	-9.9326134E 00
300.	1000.	2.3816241E 00	2.0932960E-02	-3.5658266E-05	2.8153815E-08	-8.4676533E-12	-7.1725203E 04	1.1553267E 01
MG1H1(G)		300.00	5000.00					
1000.	5000.	3.4304253E 00	1.3073366E-03	-5.4209792E-07	1.0827768E-10	-7.5970585E-15	1.9345305E 04	3.1673993E 00
300.	1000.	3.6296044E 00	-2.0758356E-03	8.4871303E-06	-8.7237306E-09	2.9791774E-12	1.9438617E 04	2.8573864E 00

MG1O1(G)		300.00	5000.00					
1000.	5000.	1.5739759E 00	5.4020523E-03	-2.5844603E-06	5.0563843E-10	-3.5393625E-14	1.6545825E 03	1.4997619E 01
300.	1000.	2.5459514E 00	7.2723352E-03	-1.2693082E-05	1.1359031E-08	-3.6224244E-12	1.1210638E 03	8.7464383E 00
MG1O1(S)		300.00	5000.00					
1000.	5000.	4.5348647E 00	2.9477999E-03	-1.7676425E-06	5.0086172E-10	-5.4331266E-14	-7.3891310E 04	-2.3649626E 01
300.	1000.	-6.4207082E-02	2.5463209E-02	-4.3992098E-05	3.6093858E-08	-1.1339213E-11	-7.3116398E 04	-2.3266586E 00
MG1O1H1(G)		300.00	5000.00					
1000.	5000.	4.5649561E 00	1.8692083E-03	-6.2089273E-07	9.8010720E-11	-5.9870911E-15	-7.6517622E 03	2.3988377E 00
300.	1000.	2.4594332E 00	1.0554265E-02	-1.3938193E-05	9.0434884E-09	-2.2136996E-12	-7.2444947E 03	1.2486970E 01
MG1S1(G)		300.00	5000.00					
1000.	5000.	4.3342079E 00	2.4779938E-04	-8.2777613E-08	1.6063989E-11	-1.1469454E-15	1.5903071E 04	2.2515730E 00
300.	1000.	3.0460532E 00	5.9294204E-03	-9.8598641E-06	7.6734301E-09	-2.2748939E-12	1.6149851E 04	8.3727337E 00
N1(G)		300.00	5000.00					
1000.	5000.	2.4398254E 00	1.2681515E-04	-8.7353204E-08	2.1962665E-11	-1.2978534E-15	5.6149884E 04	4.5062000E 00
300.	1000.	2.4922752E 00	5.7972804E-05	-1.5047617E-07	1.6213444E-10	-6.1954139E-14	5.6129985E 04	4.2127331E 00
N2(G)		300.00	5000.00					
1000.	5000.	2.8609546E 00	1.5851765E-03	-6.1779901E-07	1.1119420E-10	-7.5210614E-15	-8.9248972E 02	6.3553564E 00
300.	1000.	3.6927389E 00	-1.3411998E-03	2.6693385E-06	-9.9559574E-10	-9.3276676E-14	-1.0629498E 03	2.2827699E 00
N1F1(G)		300.00	5000.00					
1000.	5000.	3.9617527E 00	6.6673228E-04	-2.6302304E-07	5.0938003E-11	-3.6361340E-15	3.1890599E 04	2.7589592E 00
300.	1000.	2.8312862E 00	3.8325543E-03	-3.1590759E-06	7.7572379E-10	1.3227553E-13	3.2195126E 04	8.5745765E 00
N1F2(G)		300.00	5000.00					
1000.	5000.	5.7106366E 00	1.4551743E-03	-6.4178169E-07	1.2530573E-10	-9.0095639E-15	2.5583242E 03	-3.3189464E 00
300.	1000.	2.4348801E 00	1.1912004E-02	-1.2904760E-05	6.1492358E-09	-9.5103478E-13	3.3757479E 03	1.3211366E 01
N1F3(G)		300.00	5000.00					
1000.	5000.	7.9274943E 00	2.3427804E-03	-1.0323787E-06	2.0119243E-10	-1.4433841E-14	-1.7786216E 04	-1.5390800E 01
300.	1000.	4.9963812E-01	2.9671511E-02	-4.0252528E-05	2.6052026E-08	-6.5459967E-12	-1.6105738E 04	2.1216300E 01
N2F2(G)		300.00	5000.00					
1000.	5000.	8.2593877E 00	1.9801913E-03	-8.7798989E-07	1.7206650E-10	-1.2405738E-14	6.8931306E 03	-1.5738029E 01
300.	1000.	1.2225309E 00	2.9370923E-02	-4.2824597E-05	2.9828417E-08	-8.0760275E-12	8.4154602E 03	1.8583882E 01
N2F4(G)		300.00	5000.00					
1000.	5000.	1.2681045E 01	3.7601643E-03	-1.6605017E-06	3.2421997E-10	-2.3298791E-14	-5.5579566E 03	-3.8170838E 01
300.	1000.	-2.8067195E-01	5.3534438E-02	-7.6782082E-05	5.2655723E-08	-1.4045785E-11	-2.7212292E 03	2.5213831E 01
N1H1(G)		300.00	5000.00					
1000.	5000.	2.7323948E 00	1.4098251E-03	-4.5212529E-07	7.4009378E-11	-4.4819980E-15	3.8928147E 04	6.0169364E 00
300.	1000.	3.4484270E 00	5.7312325E-04	-2.0875157E-06	3.0794744E-09	-1.2538877E-12	3.8674111E 04	2.0356879E 00
N1H3(G)		300.00	5000.00					
1000.	5000.	2.1395874E 00	6.5117869E-03	-2.2818258E-06	3.7712311E-10	-2.3888154E-14	-6.3984359E 03	9.2789754E 00
300.	1000.	3.7743808E 00	-5.0670871E-04	9.9245863E-06	-9.6206360E-09	3.1511623E-12	-6.7283556E 03	1.4403369E 00
N1O1(G)		300.00	5000.00					
1000.	5000.	3.1551830E 00	1.4048594E-03	-5.6989160E-07	1.0615069E-10	-7.3658970E-15	9.8508084E 03	6.9308525E 00
300.	1000.	4.2138789E 00	-4.6222170E-03	1.1011345E-05	-9.2994568E-09	2.7853867E-12	9.7380902E 03	2.2911135E 00
N1O2(G)		300.00	5000.00					
1000.	5000.	4.6041420E 00	2.6599992E-03	-1.1092033E-06	2.1192393E-10	-1.4985575E-14	2.3853524E 03	1.4196383E 00
300.	1000.	3.4952549E 00	1.7608257E-03	7.9363390E-06	-1.1082089E-08	4.2415478E-12	2.9008426E 03	8.1564996E 00
N2O1(G)		300.00	5000.00					
1000.	5000.	4.6104152E 00	3.0533130E-03	-1.2357618E-06	2.3363675E-10	-1.6289392E-14	8.1412030E 03	-1.0594781E 00
300.	1000.	2.3981125E 00	1.0219288E-02	-1.0814929E-05	6.5703074E-09	-1.7274666E-12	8.7216412E 03	1.0161746E 01
N1S1(G)		300.00	5000.00					
1000.	5000.	3.8424980E 00	7.4172882E-04	-3.0322953E-07	5.7411333E-11	-4.0138733E-15	3.0784440E 04	4.4610909E 00
300.	1000.	4.0622151E 00	-2.8190179E-03	9.3158088E-06	-9.5089130E-09	3.2843034E-12	3.0872668E 04	4.0612628E 00
NA1(G)		300.00	5000.00					
1000.	5000.	2.4174623E 00	1.7995503E-04	-1.2744458E-07	3.1573603E-11	-1.2544430E-15	1.2315004E 04	4.6742838E 00
300.	1000.	2.5293740E 00	-2.2333869E-04	5.8917296E-07	-6.4546229E-10	2.5054600E-13	1.2284766E 04	4.1089383E 00
NA1(L)		370.98	2500.00					
1000.	5000.	2.2293458E 00	2.2240186E-03	-1.2738518E-06	3.3938162E-10	-3.4901584E-14	-1.7665257E 02	-5.7183239E 00
300.	1000.	4.5761129E 00	-2.5390745E-03	1.4497210E-06	-0.	-0.	-9.7542442E 02	-1.8451459E 01
NA1(S)		300.00	370.98					
1000.	5000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
300.	1000.	1.6829897E 00	1.4682614E-02	-5.2049962E-05	7.4260785E-08	-0.	-8.4124353E 02	-6.1499926E 00
NA2(G)		300.00	5000.00					
1000.	5000.	4.4816540E 00	2.2315443E-04	-1.1531490E-08	2.4575841E-12	-1.8965185E-16	1.5695871E 04	2.0623236E 00
300.	1000.	4.2998955E 00	1.0510880E-03	-1.4378583E-06	1.0901677E-09	-3.0774814E-13	1.5728689E 04	2.9174162E 00
NA1CL1(G)		300.00	5000.00					
1000.	5000.	4.4260228E 00	1.6777751E-04	-3.0996042E-08	5.4328400E-12	-3.4959106E-16	-2.3241252E 04	2.2961729E 00
300.	1000.	3.5818939E 00	4.0450981E-03	-6.9457741E-06	5.5826335E-09	-1.6959647E-12	-2.3086035E 04	6.2721135E 00
NA2CL2(G)		300.00	5000.00					
1000.	5000.	9.7992842E 00	2.4470324E-04	-1.1473532E-07	2.3516530E-11	-1.7578663E-15	-7.1776153E 04	-1.7046902E 01
300.	1000.	7.6417366E 00	1.0630669E-02	-1.9345980E-05	1.6019731E-08	-4.9951489E-12	-7.1401550E 04	-6.9971598E 00
NA1F1(G)		300.00	5000.00					
1000.	5000.	4.3320317E 00	2.6411754E-04	-8.4645588E-08	1.6489458E-11	-1.1809987E-15	-3.6872016E 04	1.2154635E 00
300.	1000.	3.0467419E 00	5.9100445E-03	-9.7501857E-06	7.5417007E-09	-2.2214902E-12	-3.6625084E 04	7.3274472E 00
NA2F2(G)		300.00	5000.00					
1000.	5000.	9.6989263E 00	3.5190302E-04	-1.5859262E-07	3.1398936E-11	-2.2788458E-15	-1.0579889E 05	-1.9524392E 01
300.	1000.	6.4571786E 00	1.5685877E-02	-2.8156167E-05	2.3054757E-08	-7.1202914E-12	-1.0522384E 05	-4.3613296E 00
NA1H1(G)		300.00	5000.00					
1000.	5000.	3.7957045E 00	8.9082140E-04	-3.3472808E-07	6.4226210E-11	-4.5502470E-15	1.3607882E 04	5.6523558E-01
300.	1000.	3.1501344E 00	1.2050952E-03	2.6519336E-06	-4.4145020E-09	1.8188135E-12	1.3855770E 04	4.2541407E 00
NA1O1(G)		300.00	5000.00					
1000.	5000.	4.2398042E 00	3.5864951E-04	-1.2843692E-07	2.4834200E-11	-1.7675778E-15	5.3149838E 03	2.1065041E 00
300.	1000.	2.7675754E 00	6.3739320E-03	-9.7471759E-06	7.0671271E-09	-1.9683760E-12	5.6185660E 03	9.2146077E 00
NA1O1H1(G)		300.00	5000.00					
1000.	5000.	4.7714693E 00	1.6424058E-03	-5.2387121E-07	7.9624403E-11	-4.7010912E-15	-2.9617935E 04	8.5785822E-01
300.	1000.	3.1188732E 00	9.1706713E-03	-1.2997836E-05	9.0243381E-09	-2.3511211E-12	-2.9338379E 04	8.5873367E 00
NA1O1H1(L)		592.30	2500.00					
1000.	5000.	1.0069140E 01	-0.	-0.	-0.	-0.	-5.4086818E 04	-4.8132426E 01
300.	1000.	1.0773628E 01	-7.0448759E-04	-0.	-0.	-0.	-5.4439060E 04	-5.2294366E 01
NA1O1H1(S)		300.00	566.00					
1000.	5000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
300.	1000.	8.6474341E 00	-1.3402397E-02	2.8384837E-05	-0.	-0.	-5.3681028E 04	-3.8816109E 01

NA1O1H1(S)		566.00	592.30					
1000.	5000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
300.	1000.	1.0345903E 01	-0.	-0.	-0.	-0.	-5.4309095E 04	-5.1270542E 01
NA2O2H2(G)		300.00	5000.00					
1000.	5000.	1.0482111E 01	4.4723966E-03	-1.5661649E-06	2.5941072E-10	-1.6532703E-14	-8.7331067E 04	-2.4392795E 01
300.	1000.	3.6887952E 00	3.2195651E-02	-4.4597800E-05	3.0140996E-08	-7.7964254E-12	-8.5969919E 04	8.3107708E 00
NE1(G)		300.00	5000.00					
1000.	5000.	2.4987054E 00	1.8317316E-06	-9.6258649E-10	2.1654450E-13	-1.7473877E-17	6.8614251E-01	3.3497911E 00
300.	1000.	2.4728945E 00	2.0491592E-04	-5.3678938E-07	5.8390785E-10	-2.2515537E-13	2.6685684E 00	3.4546362E 00
O1(G)		300.00	5000.00					
1000.	5000.	2.5372567E 00	-1.8422190E-05	-8.8017921E-09	5.9643621E-12	-5.5743608E-16	2.9230007E 04	4.9467942E 00
300.	1000.	3.0218894E 00	-2.1737249E-03	3.7542203E-06	-2.9947200E-09	9.0777547E-13	2.9137190E 04	2.6460076E 00
O2(G)		300.00	5000.00					
1000.	5000.	3.5980995E 00	7.8056719E-04	-2.2337506E-07	4.2396622E-11	-3.3419056E-15	-1.1929753E 03	3.7465771E 00
300.	1000.	3.7189946E 00	-2.5167288E-03	8.5837353E-06	-8.2998716E-09	2.7082180E-12	-1.0576706E 03	3.9080704E 00
O1H1(G)		300.00	5000.00					
1000.	5000.	2.9029511E 00	9.7345968E-04	-2.0321080E-07	1.5911612E-11	-5.1673895E-17	3.8779933E 03	5.4854499E 00
300.	1000.	3.8424287E 00	-1.2668453E-03	1.6504889E-06	-6.6768888E-10	1.3067663E-13	3.5855228E 03	5.0440906E-01
P1(G)		300.00	5000.00					
1000.	5000.	2.6258122E 00	-1.6768917E-04	6.6485428E-09	4.1060775E-11	-5.7533818E-15	3.7032311E 04	4.6539916E 00
300.	1000.	2.5016955E 00	-1.3327000E-05	3.6614834E-08	-4.1852754E-11	1.6948331E-14	3.7085446E 04	5.3639764E 00
P2(G)		300.00	5000.00					
1000.	5000.	4.1440200E 00	4.2981666E-04	-1.7589353E-07	3.3655387E-11	-2.3331858E-15	1.5505858E 04	2.3200494E 00
300.	1000.	2.6943141E 00	5.8599281E-03	-8.0869497E-06	5.3041531E-09	-1.3421810E-12	1.5827871E 04	9.4378082E 00
S1(G)		300.00	5000.00					
1000.	5000.	2.9077021E 00	-5.5374975E-04	2.7763294E-07	-5.0125621E-11	3.1270093E-15	3.2607656E 04	3.8020261E 00
300.	1000.	2.8649268E 00	6.5186070E-04	-3.4354430E-06	3.9874975E-09	-1.4842559E-12	3.2573389E 04	3.7744064E 00
S1(S)		300.00	388.36					
1000.	5000.	0.	0.	0.	0.	0.	0.	0.
300.	1000.	-1.8402765E 00	3.3260648E-02	-7.3745724E-05	2.5754883E-08	6.6031132E-11	-3.6015645E 02	7.3248802E 00
S2(G)		300.00	5000.00					
1000.	5000.	4.1896932E 00	3.8469704E-04	-1.5566633E-07	3.0368010E-11	-2.1795849E-15	1.4188133E 04	3.2930300E 00
300.	1000.	2.6999349E 00	6.2749549E-03	-9.2870775E-06	6.5393276E-09	-1.7802282E-12	1.4504935E 04	1.0534222E 01
S1CL1(G)		300.00	5000.00					
1000.	5000.	4.3335924E 00	2.5773749E-04	-8.2783921E-08	1.6021290E-11	-1.1403914E-15	1.4957786E 04	3.2509732E 00
300.	1000.	3.0477836E 00	5.9037752E-03	-9.7474366E-06	7.5404658E-09	-2.2211620E-12	1.5205019E 04	9.3661710E 00
S1CL2(G)		300.00	5000.00					
1000.	5000.	6.6442166E 00	4.1085430E-04	-1.8366739E-07	3.6163024E-11	-2.6144755E-15	-4.6798654E 03	-4.3190122E 00
300.	1000.	3.7909214E 00	1.3180560E-02	-2.2438298E-05	1.7654212E-08	-5.2824457E-12	-4.1417595E 03	9.1957369E 00
S2CL2(G)		300.00	5000.00					
1000.	5000.	9.5051272E 00	5.6684538E-04	-2.5099070E-07	4.8952275E-11	-3.5081484E-15	-3.3950071E 03	-1.5455237E 01
300.	1000.	5.0882460E 00	2.0810339E-02	-3.6366951E-05	2.9280534E-08	-8.9457457E-12	-2.5806676E 03	5.3616804E 00
S1F1(G)		300.00	5000.00					
1000.	5000.	4.0905957E 00	5.0956359E-04	-2.0130365E-07	3.9007849E-11	-2.7846707E-15	3.2756220E 02	3.0147026E 00
300.	1000.	2.7368470E 00	5.1142157E-03	-6.0734591E-06	3.2886491E-09	-6.3117417E-13	6.4963762E 02	9.7713761E 00
S1F2(G)		300.00	5000.00					
1000.	5000.	6.0466650E 00	1.0773709E-03	-4.7443582E-07	9.2386330E-11	-6.6227946E-15	-3.2167428E 04	-4.2777185E 00
300.	1000.	2.5990880E 00	1.3695181E-02	-1.8466121E-05	1.1866766E-08	-2.9595516E-12	-3.1384537E 04	1.2728771E 01
S1F6(G)		300.00	5000.00					
1000.	5000.	1.5245670E 01	4.2781334E-03	-1.8957742E-06	3.7096750E-10	-2.6696924E-14	-1.5067551E 05	-5.4851048E 01
300.	1000.	-3.3342495E 00	7.9620210E-02	-1.2204395E-04	8.8573794E-08	-2.4843513E-11	-1.4680458E 05	3.5029756E 01
S2F2(G)		300.00	5000.00					
1000.	5000.	8.7904583E 00	1.3701365E-03	-6.0388189E-07	1.1760841E-10	-8.4290287E-15	-3.4624636E 04	-1.4848331E 01
300.	1000.	3.1478452E 00	2.3926502E-02	-3.6082882E-05	2.5835446E-08	-7.1610225E-12	-3.3432814E 04	1.2528128E 01
S1O1(G)		300.00	5000.00					
1000.	5000.	3.8116451E 00	7.8966107E-04	-3.2986127E-07	6.3513293E-11	-4.5139892E-15	-5.9599488E 02	4.5442232E 00
300.	1000.	3.1364326E 00	1.3080689E-03	2.1837364E-06	-3.9518236E-09	1.6540306E-12	-3.4572672E 02	8.3570292E 00
S1O2(G)		300.00	5000.00					
1000.	5000.	5.1982451E 00	2.0595095E-03	-8.6254450E-07	1.6636523E-10	-1.1847837E-14	-3.7541457E 04	-8.3059963E-01
300.	1000.	3.2257132E 00	5.6551207E-03	-2.4970208E-07	-4.2206766E-09	2.1392733E-12	-3.6904476E 04	9.8177036E 00
S1O3(G)		300.00	5000.00					
1000.	5000.	6.8889555E 00	4.2828041E-03	-1.4859365E-06	2.8594348E-10	-2.0314293E-14	-5.0167044E 04	-1.0598504E 01
300.	1000.	1.7692057E 00	1.8576331E-02	-1.4957361E-05	4.3746772E-09	1.8859868E-13	-4.8767551E 04	1.5794520E 01
S1O1CL1(G)		300.00	5000.00					
1000.	5000.	5.9491040E 00	1.1688403E-03	-5.0955147E-07	9.8542227E-11	-7.0288320E-15	-1.4550197E 04	-9.1362507E-01
300.	1000.	3.5171217E 00	9.4362547E-03	-1.1447975E-05	6.7641889E-09	-1.5696850E-12	-1.3959661E 04	1.1256492E 01
S1O1CL2(G)		300.00	5000.00					
1000.	5000.	8.7881265E 00	1.3682553E-03	-6.0395837E-07	1.1802732E-10	-8.4934617E-15	-2.8582896E 04	-1.3886094E 01
300.	1000.	4.4329079E 00	1.8705595E-02	-2.8019371E-05	2.0259954E-08	-5.7171315E-12	-2.7651631E 04	7.2822402E 00
S1O1F1(G)		300.00	5000.00					
1000.	5000.	5.6379891E 00	1.5167400E-03	-6.6184797E-07	1.2810434E-10	-9.1446735E-15	-1.6982878E 04	-1.0800061E 00
300.	1000.	2.9497184E 00	9.3823361E-03	-8.6590471E-06	3.0509610E-09	-1.1212771E-13	-1.6271790E 04	1.2674373E 01
S1O1F2(G)		300.00	5000.00					
1000.	5000.	8.0366592E 00	2.2000212E-03	-9.6412190E-07	1.8717774E-10	-1.3391199E-14	-5.6045995E 04	-1.3660891E 01
300.	1000.	1.7914919E 00	2.5459879E-02	-3.5068531E-05	2.3342059E-08	-6.0785565E-12	-5.4638309E 04	1.7069540E 01
S1O2F2(G)		300.00	5000.00					
1000.	5000.	9.5354137E 00	3.8605982E-03	-1.6873173E-06	3.2717781E-10	-2.3395576E-14	-1.0665259E 05	-2.2471018E 01
300.	1000.	9.6315531E-01	3.3955964E-02	-4.3049634E-05	2.6612969E-08	-6.4699807E-12	-1.0462271E 05	2.0179552E 01
SI1(G)		300.00	5000.00					
1000.	5000.	2.6590261E 00	-3.7411807E-04	3.0631825E-07	-7.5405128E-11	6.0200418E-15	5.2254730E 04	5.1745855E 00
300.	1000.	3.3120935E 00	-3.7036043E-03	6.8103371E-06	-5.7141250E-09	1.8171407E-12	5.2145855E 04	2.1676254E 00
SI1(L)		1685.00	5000.00					
1000.	5000.	3.1133319E 00	-0.	-0.	-0.	-0.	5.1623365E 03	-1.2076148E 01
300.	1000.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
SI1(S)		300.00	1685.00					
1000.	5000.	7.9656259E-01	6.1706699E-03	-6.2931271E-06	3.0775881E-09	-5.6171799E-13	-3.8786628E 02	-3.6953660E 00
300.	1000.	3.4558844E-01	1.1713164E-02	-2.0789535E-05	1.7372252E-08	-5.4514965E-12	-4.7171395E 02	-2.4168814E 00
SI2(G)		300.00	5000.00					
1000.	5000.	4.3450344E 00	2.2261486E-04	-7.6286371E-08	1.4678435E-11	-1.0391791E-15	7.2930682E 04	2.7210055E 00
300.	1000.	3.0731227E 00	5.9325545E-03	-1.0095074E-05	8.0214356E-09	-2.4270378E-12	7.3170729E 04	8.7440939E 00

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SI3(G)                 300.00    5000.00
 1000.  5000.   7.0880004E 00   4.7014225E-04  -2.0758091E-07   4.0394582E-11  -2.8895204E-15   7.7534916E 04  -1.0264577E 01
  300.  1000.   3.6720107E 00   1.5889358E-02  -2.7344845E-05   2.1745958E-08  -6.5744189E-12   7.8174967E 04   5.8893536E 00

SI1CL1(G)              300.00    5000.00
 1000.  5000.   4.4178274E 00   1.3112192E-04  -3.2742526E-08   5.4972693E-12  -3.3022321E-16   2.2660741E 04   3.2772562E 00
  300.  1000.   3.7783602E 00   2.8341376E-03  -4.5116467E-06   3.3987709E-09  -9.7824888E-13   2.2788933E 04   6.3443629E 00

SI1CL2(G)              300.00    5000.00
 1000.  5000.   6.5858971E 00   4.7180808E-04  -2.0823663E-07   4.0531052E-11  -2.9007437E-15  -2.2717268E 04  -4.2997550E 00
  300.  1000.   3.5203741E 00   1.3999387E-02  -2.3561504E-05   1.8431707E-08  -5.5028670E-12  -2.2128913E 04   1.0269781E 01

SI1CL4(G)              300.00    5000.00
 1000.  5000.   1.2077901E 01   1.0672182E-03  -4.7852424E-07   9.4504402E-11  -6.8513637E-15  -7.7186275E 04  -2.9874038E 01
  300.  1000.   5.2798827E 00   3.1117379E-02  -5.2302685E-05   4.0775397E-08  -1.2115730E-11  -7.5887065E 04   2.4138489E 00

SI1F1(G)               300.00    5000.00
 1000.  5000.   4.1276518E 00   4.6295701E-04  -1.8389672E-07   3.5099066E-11  -2.3624693E-15   1.0808561E 03   3.3489127E 00
  300.  1000.   3.2635203E 00   2.8480547E-03  -2.1898874E-06   2.6472977E-10   2.5303142E-13   1.3126160E 03   7.7956275E 00

SI1F2(G)               300.00    5000.00
 1000.  5000.   5.7664934E 00   1.3819963E-03  -6.0505245E-07   1.1732992E-10  -8.3844494E-15  -6.3718807E 04  -3.1468068E 00
  300.  1000.   2.6998288E 00   1.1038411E-02  -1.1713626E-05   5.4063594E-09  -7.7859148E-13  -6.2945708E 04   1.2364374E 01

SI1F4(G)               300.00    5000.00
 1000.  5000.   1.0492797E 01   2.8310884E-03  -1.2475869E-06   2.4324435E-10  -1.7461290E-14  -1.9233078E 05  -2.7671199E 01
  300.  1000.   2.3901709E 00   3.1982032E-02  -4.1995237E-05   2.6299933E-08  -6.3748200E-12  -1.9046378E 05   1.2426418E 01

SI1H1(G)               300.00    5000.00
 1000.  5000.   3.0314187E 00   1.5528097E-03  -6.0921584E-07   1.1293413E-10  -7.8132836E-15   4.3959998E 04   6.1333672E 00
  300.  1000.   3.8413117E 00  -2.7362435E-03   6.9981472E-06  -5.5238444E-09   1.5007631E-12   4.3866323E 04   2.5259783E 00

SI1H4(G)               300.00    5000.00
 1000.  5000.   4.2864439E 00   8.9421998E-03  -3.7030738E-06   6.9171116E-10  -4.8137695E-14   1.9035952E 03  -3.1698731E 00
  300.  1000.   1.6111312E 00   1.2719990E-02  -1.6884339E-06  -4.5135745E-09   2.0400319E-12   2.9021544E 03   1.1738476E 01

SI1N1(G)               300.00    5000.00
 1000.  5000.   3.8063403E 00   7.9712358E-04  -3.3158207E-07   6.2840384E-11  -4.2600825E-15   5.9042866E 04   3.9540278E 00
  300.  1000.   3.1471330E 00   1.2265928E-03   2.3774131E-06  -4.1441265E-09   1.7234504E-12   5.9290539E 04   7.6940989E 00

SI1O1(G)               300.00    5000.00
 1000.  5000.   3.7295164E 00   8.6335951E-04  -3.5894469E-07   6.8212796E-11  -4.7844561E-15  -1.2008310E 04   3.7472829E 00
  300.  1000.   3.3495882E 00  -2.6538250E-04   5.4814021E-06  -6.8793292E-09   2.6110821E-12  -1.1797081E 04   6.2421835E 00

SI1O2(G)               300.00    5000.00
 1000.  5000.   5.6085578E 00   2.0706559E-03  -8.9489692E-07   1.7221365E-10  -1.2248362E-14  -3.8838927E 04  -5.6134425E 00
  300.  1000.   3.0434082E 00   9.6089730E-03  -9.1104569E-06   4.0471334E-09  -6.4477587E-13  -3.8146640E 04   7.5419379E 00

SI1S1(G)               300.00    5000.00
 1000.  5000.   4.1728212E 00   3.9618379E-04  -1.5985232E-07   3.0306992E-11  -2.0739258E-15   1.3354838E 04   2.8391688E 00
  300.  1000.   2.6860287E 00   6.1744527E-03  -8.9647337E-06   6.2071096E-09  -1.6654723E-12   1.3675935E 04   1.0090654E 01

END    000000000000     0.         0.
    0.      0.    0.            0.              0.              0.              0.              0.              0.
    0.      0.    0.            0.              0.              0.              0.              0.              0.
```

APPENDIX C

PROGRAM LISTING FOR IBM 704

```
C     MAIN PROGRAM ONE
C
C
      COMMON C
      EQUIVALENCE   (G(1),       C(1)),      (G(420),     C(420))
      EQUIVALENCE   (FORM(1),    C(1)),      (FORM(15),   C(15))
      EQUIVALENCE   (ELMT(1),    C(16)),     (ELMT(15),   C(30))
      EQUIVALENCE   (DATA(1),    C(31)),     (DATA(23),   C(53))
      EQUIVALENCE   (A(1),       C(421)),    (A(1350),    C(1770))
      EQUIVALENCE   (COEFT(1),   C(421)),    (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),     C(421)),    (ANS(454),   C(874))
      EQUIVALENCE   (HSUM,       C(424)),    (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,      C(426)),    (CP,         C(427))
      EQUIVALENCE   (DLMPT,      C(428)),    (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,      C(430)),    (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,      C(432)),    (SP IMP,     C(433))
      EQUIVALENCE   (VACI,       C(434)),    (CF,         C(436))
      EQUIVALENCE   (RHOI,       C(437)),    (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),    (PI I,       C(441))
      EQUIVALENCE   (EP PI,      C(442)),    (AW PI,      C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),    (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,     C(448)),    (T SIG,      C(450))
      EQUIVALENCE   (SIG I,      C(451)),    (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQ'JIVALENCE  (EN(1),      C(1771)),   (EN(90),     C(1860))
      EQUIVALENCE   (BOX(1),     C(1771)),   (BOX(15),    C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)),   (BOF(15),    C(1800))
      EQUIVALENCE   (HX,         C(1801)),   (HF,         C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)),   (VXMIN,      C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)),   (VFMIN,      C(1806))
      EQUIVALENCE   (EN LN(1),   C(1861)),   (EN LN(90),  C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)),   (DEL N(90),  C(2040))
      EQUIVALENCE   (COEFX(1),   C(1951)),   (COEFX(20),  C(1970))
      EQUIVALENCE   (DX(1),      C(1951)),   (DX(20),     C(1970))
      EQUIVALENCE   (HO(1),      C(2041)),   (HO(90),     C(2130))
      EQUIVALENCE   (S(1),       C(2131)),   (S(90),      C(2220))
      EQUIVALENCE   (X(1),       C(2221)),   (X(20),      C(2240))
      EQUIVALENCE   (FORMLA(1),  C(2221)),   (FORMLA(18), C(2238))
      EQUIVALENCE   (DELTA(1),   C(2241)),   (DELTA(20),  C(2260))
      EQUIVALENCE   (BO(1),      C(2261)),   (BO(15),     C(2275))
      EQUIVALENCE   (PO,         C(2276)),   (HSUBO,      C(2277))
      EQUIVALENCE   (SO,         C(2278)),   (T LN,       C(2279))
      EQUIVALENCE   (T,          C(2280)),   (AAY LN,     C(2281))
      EQUIVALENCE   (AAY,        C(2282)),   (CPSUM,      C(2283))
      EQUIVALENCE   (HC,         C(2284)),   (TC LN,      C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)),   (PCP(25),    C(2310))
      EQUIVALENCE   (PROD(1),    C(2311)),   (PROD(3),    C(2313))
      EQUIVALENCE   (DATUM(1),   C(2311)),   (DATUM(3),   C(2313))
      EQUIVALENCE   (PC,         C(2314)),   (TC,         C(2315))
      EQUIVALENCE   (IPROB,      C(2316)),   (IFIXT,      C(2317))
      EQUIVALENCE   (IHS,        C(2318)),   (ICOND,      C(2319))
      EQUIVALENCE   (ISYM,       C(2320)),   (IPROD,      C(2321))
      EQUIVALENCE   (IDID,       C(2322)),   (LDRUM,      C(2323))
      EQUIVALENCE   (IDRM,       C(2323)),   (KDRUM,      C(2324))
      EQUIVALENCE   (L,          C(2325)),   (L1,         C(2326))
      EQUIVALENCE   (M,          C(2327)),   (M1,         C(2328))
      EQUIVALENCE   (N,          C(2329)),   (IO,         C(2330))
      EQUIVALENCE   (IO1,        C(2331)),   (IO2,        C(2332))

      EQUIVALENCE   (IO3,        C(2333)),   (KMAT,       C(2334))
      EQUIVALENCE   (IMAT,       C(2335)),   (IUSE,       C(2335))
      EQUIVALENCE   (IADD,       C(2336)),   (ITNUMB,     C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)),   (P,          C(2339))
      EQUIVALENCE   (IDEBUG,     C(2340)),   (IFROZ,      C(2341))
C
      DIMENSION   G(20,21),    A(15,90),     EN(90),       EN LN(90)
      DIMENSION   DEL N(90),   HO(90),       S(90),        X(20)
      DIMENSION   DELTA(20),   BO(15),       PCP(25),      PROD(3)
      DIMENSION   COEFX(20),   DX(20),       FORM(15),     COEFT(15,90)
      DIMENSION   ELMT(15),    DATA(23),     DATUM(3),     FORMLA(18)
      DIMENSION   BOX(15),     BOF(15),      ANS(454),     SYSTM(15)
C
C
S H S ALF   H,S
S T S ALF   T,S
S P T ALF   P,T
S T P ALF   T,P
S DET ALF   DETN
S END ALF   END
S BLK ALF   00000
SOMIT ALF   OMIT
S MT  ALF
C
C     CONVERT BST TO BSF INSTRUCTIONS AT 450,1457,531,596,600,225,229
C
S 390 CAL*390
S     STP*450
S     STP*1457
S     STP*531
S     STP*596
S     STP*600
S     STP*225
S     STP*229
C
C     READ IN INPUT DATA
C
  400 READ DRUM 4,455,ISYS
      IF (ISYS-99) 401,403,401
  403 READ TAPE 3,(G(I),I=1,2341)
      REWIND 3
      IF (SENSE SWITCH 6) 651,719
  401 ISYS=99
      WRITE DRUM 4,455,ISYS
      IFROZ=0
      PAUSE 11111
  405 I3=3
      I4=4
      KDRUM=2
      LDRUM=3
      ITAPE=4
  429 CALL INPUT
      IF (L) 651,651,433
  433 WRITE OUTPUT TAPE 6,443, HX,VXPLS,VXMIN,HF,VFPLS,VFMIN
     1, (ELMT(I),BOX(I),BOF(I),I=1,L)
  443 FORMAT (10H1OXIDANT  3E16.6/10H FUEL      3E16.6/(1H A6,2E20.8))
C
C     RIGHT ADJUST ELEMENT SYMBOLS
C
      DO 447 K=1,L
```

```
S       CLM
S       SSP
S       LDQ ELMT(K)
S       LGL 12
S       STO ELMT(K)
S       LRS 6
S       CLM
S       LLS 6
S       SUB BLK
S       TNZ*447
S       CLA ELMT(K)
S       LRS 6
S       STO ELMT(K)
  447 CONTINUE
      READ DRUM 4,456,SYSTM
S       CLA SYSTM(L+1)
S       TNZ*453
S       CLA SYSTM(L)
S       TZE*453
      DO 449 K=1,L
      DO 448 J=1,L
S       CLA ELMT(K)
S       SUB SYSTM(J)
S       TZE*449
  448 CONTINUE
      GO TO 453
  449 CONTINUE
      REWIND I3
S 450 BST 4
S       NOP
S       RTB 4
C
C     CANCEL ---OMITS---FROM PREVIOUS PROBLEM
C
  452 DO 1455 INT=1,2
      READ TAPE ITAPE,((COEFT(K,J),K=1,15),J=1,90)
      DO 1453 J=1,M
S       CLA MT
S1453 STO COEFT(1,J)
 1455 WRITE TAPE 3,((COEFT(K,J),K=1,15),J=1,90)
      IUSE=1
      REWIND 3
S1457 BST 4
S       NOP
S       RTB 4
      GO TO 598
  453 DO 459 K=1,15
  459 SYSTM(K)=ELMT(K)
      WRITE DRUM 4,456,SYSTM
      ITAPE=2
      REWIND I3
      REWIND I4
C
C     BYPASS PING-PONG CORE LOADS ON TAPE 2 AND SAVE MASTER DATA FROM
C     TAPE 4 ON TAPE 2
C
C
S 522 RTB 2
S       CPY
S       TRA*522

S       TRA*523
S       TRA*522
  523 READ TAPE I4, (DATA(I),I=1,23)
      WRITE TAPE 2, (DATA(I),I=1,23)
S       CLA DATA(1)
S       SUB END
S       TNZ*523
S 531 BST 2
S       NOP
S       RTB 2
      REWIND I3
      REWIND I4
      CALL SEARCH(I3,I4,IUSE)
C
C     PUT COMPILED DATA TAPE ON TAPE 4 FOLLOWING MASTER DATA
C
  591 IF (I4-4) 596,593,596
  593 DO 594 INT=1,2
      READ TAPE I4,((COEFT(K,J),K=1,15),J=1,90)
      WRITE TAPE I3,((COEFT(K,J),K=1,15),J=1,90)
  594 CONTINUE
      REWIND I3
      REWIND I4
S 596 BST 2
S       NOP
S       RTB 2
  597 READ TAPE ITAPE,(DATA(I),I=1,23)
      WRITE TAPE 4, (DATA(I),I=1,23)
S       CLA DATA(1)
S       SUB END
S       TNZ*597
      END FILE 4
  598 DO 599 INT=1,2
      READ TAPE  3,((COEFT(K,J),K=1,15),J=1,90)
  599 WRITE TAPE 4,((COEFT(K,J),K=1,15),J=1,90)
      IF (IUSE-2) 600,635,635
S 600 BST 4
S       NOP
S       RTB 4
      REWIND 3
C
C     SET ARRAY  PROD  TO BYPASS ALL CONDENSED PHASES
C
      PROD(1)=0.0
      PROD(2)=0.0
S 197 LXD M,(M)
S       CLM
S       SSP
S       COM
S       LRS 35
S       CLM
S       TXL*198,(M),35
S       TXL*199,(M),70
S       TXL*200,(M),90
      GO TO 635
S 198 STQ PROD(3)
S       STQ PROD(2)
S       LLS 35,(M)
S       STO PROD(1)
      GO TO 201
```

```
S 199 STQ PROD(3)
S     LLS 70,(M)
S     STO PROD(2)
      GO TO 201
S 200 LLS 105,(M)
S     STO PROD(3)
  201 IQ=L
      IQ1=IQ+1
      IQ2=IQ1+1
      IQ3=IQ2+1
      L1=IQ1
      M1=M+1
C
C     DETERMINE WHICH GASEOUS SPECIES SHOULD BE OMITTED FROM THE PROBLEM
C     AND WHICH CONDENSED SPECIES SHOULD BE USED IN THE FIRST ITERATION
C
  203 READ INPUT TAPE 7,204,(DATA(I),I=1,8)
  204 FORMAT (4(2A6,3X))
S 205 CAL MT
S     COM
S     ANA DATA(1)
S     TZE*220
      DO 213 K=1,4
  207 DO 211 J=1,N
      DO 208 I=2,3
      KK=2*K+I-3
S     CAL COEFT(I,J)
S     COM
S     ANA DATA(KK)
S     TNZ*211
  208 CONTINUE
      IF (J-M) 209,209,210
  209 CALL BYPASS (J,2)
      GO TO 213
  210 CALL BYPASS (J,3)
      GO TO 213
  211 CONTINUE
  213 CONTINUE
      GO TO 203
  220 DO 224 INT=1,2
      READ TAPE 4, ((COEFT(K,J),K=1,15),J=1,90)
      DO 222 J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 221,222,221
S 221 CLA OMIT
S     STO COEFT(1,J)
  222 CONTINUE
  224 WRITE TAPE 3, ((COEFT(K,J),K=1,15),J=1,90)
      REWIND 3
S 225 BST 4
S     NOP
S     RTB 4
      DO 227 INT=1,2
      READ TAPE 3, ((COEFT(K,J),K=1,15),J=1,90)
  227 WRITE TAPE 4, ((COEFT(K,J),K=1,15),J=1,90)
      REWIND 3
S 229 BST 4
S     NOP
S     RTB 4
C

C     ARRANGE ANSWER REGION
C
      I=1
      DO 602 J=1,N
      COEFT(I)=COEFT(1,J)
      COEFT(I+1)=COEFT(2,J)
      COEFT(I+2)=COEFT(3,J)
      COEFT(I+3)=0.0
  602 I=I+4
      K=4*N
  605 I=K+34
      COEFT(I)=COEFT(K)
      K=K-1
      IF (K) 651,607,605
  607 DO 609 K=1,34
  609 COEFT(K)=0.0
      WRITE DRUM KDRUM,1576,ANS
      REWIND 2
      READ TAPE 2
      ITAPE=4
      READ TAPE ITAPE, ((COEFT(K,J),K=1,15),J=1,90)
      WRITE DRUM KDRUM,1,COEFT
C
C     DETERMINE THE TYPE OF PROBLEM
C
  700 IFROZ=1
  701 READ INPUT TAPE 7,703,PROB,KASE
  703 FORMAT (A5,I5)
      WRITE DRUM 4,789,KASE
S     CLA PROB
S     SUB H S
S     TNZ*705
      IPROB=1
      GO TO 715
S 705 ADD H S
S     SUB T S
S     TNZ*707
      IPROB=2
      GO TO 715
S 707 ADD T S
S     SUB P T
S     TNZ*709
      IPROB=3
      GO TO 715
S 709 ADD P T
S     SUB T P
S     TNZ*711
      IPROB=4
      GO TO 715
S 711 ADD T P
S     SUB DET
S     TNZ*713
      IPROB=1
      IFROZ=-1
      GO TO 719
S 713 ADD DET
S     SUB MT
S     TNZ*631
      GO TO 405
  715 DO 716 K=1,25
```

```
  716 PCP(K)=0.0
      I=0
 1716 READ INPUT TAPE 7,718,(G(K),K=1,5)
      IF (G(1)) 719,719,717
  717 DO 1717 K=1,5
      IK=I+K
 1717 PCP(IK)=G(K)
      I=I+5
      GO TO 1716
  718 FORMAT (5F10.2)
C
C     DETERMINE THE ASSIGNED VALUES FOR THE PROBLEM
C
  719 READ INPUT TAPE 7,721,EQRAT,O F,F PCT,PC,TC,KODE,IDEBUG
  721 FORMAT (5F10.2,I5,16X,I1)
      WRITE DRUM 4,482,KODE
  722 READ DRUM LDRUM,1996,BOX,BOF,HX,VXPLS,VXMIN,HF,VFPLS,VFMIN
      IF (EQRAT) 725,725,723
  723 O F=(-EQRAT*VFMIN-VFPLS)/(VXPLS+EQRAT*VXMIN)
      F PCT=100.0/(1.0+O F)
      GO TO 745
  725 IF (O F) 731,731,727
  727 F PCT=100.0/(1.0+O F)
  729 EQRAT=ABSF((O F*VXPLS+VFPLS)/(O F*VXMIN+VFMIN))
      GO TO 745
  731 IF (F PCT) 700,700,733
  733 O F=(100.0-F PCT)/F PCT
      GO TO 729
  745 IF (O F) 719,746,746
  746 DO 747 I=1,L
  747 BO(I)=(O F*BOX(I)+BOF(I))/(1.0+O F)
      IF (IPROB-1) 651,749,748
  748 HSUBO=0.0
      GO TO 755
  749 HSUBO=(O F*HX+HF)/(1.0+O F)
  755 WRITE DRUM 4,790,O F,F PCT,EQRAT
      READ DRUM 4,789,KASE
      WRITE OUTPUT TAPE 6,760,KASE,PROB,O F,F PCT,EQRAT,PC,HSUBO,
     1 (BO(I),I=1,L)
  760 FORMAT (1H1I5,3X,A6/1H 4E17.8/(1H 7E17.8))
      WRITE DRUM 4,1700,N,IPROB,BOX,BOF,BO
      HSUBO=HSUBO/1.98726
      READ DRUM LDRUM,2032,RHOX,RHOF
      READ DRUM KDRUM,1576,ANS
      RHO=RHOX+O F*RHOF
      IF (RHO) 772,772,771
  771 RHO=(1.0+O F)*RHOX*RHOF/RHO
  772 WRITE DRUM KDRUM,1576,ANS
  775 IF (IFROZ) 777,651,779
  777 CALL PONG(4)
  779 CALL PONG(2)
C
C     ERROR PRINT OUT
C
  631 WRITE OUTPUT TAPE 6,633,PROB,KASE
  633 FORMAT (21H1THERE IS NO PROBLEM A6,2X,I5)
      GO TO 651
  635 WRITE OUTPUT TAPE 6,637
  637 FORMAT (47H1TROUBLE IN COMPILING MASTER THERMODYNAMIC TAPE)
      REWIND 4

  639 READ TAPE 4,(DATA(I),I=1,23)
      WRITE OUTPUT TAPE 6,640,(DATA(I),I=1,23)
  640 FORMAT (1H 3A6,2F10.1/(1H 2F8.1,7E14.6))
S     CLA DATA(1)
S     SUB END
S     TNZ*639
      DO 641 INT=1,2
      READ TAPE 4,((COEFT(K,J),K=1,15),J=1,90)
  641 WRITE OUTPUT TAPE 6,643,((COEFT(K,J),K=1,14),J=1,N)
  643 FORMAT (1H 3A6,2F15.2/2F8.1,7E12.4//)
  651 REWIND 4
      PAUSE 77777
```

```
      SUBROUTINE SEARCH (I3,I4,JEER)
C
C
      COMMON C
      EQUIVALENCE    (G(1),        C(1)),     (G(420),     C(420))
      EQUIVALENCE    (FORM(1),     C(1)),     (FORM(15),   C(15))
      EQUIVALENCE    (ELMT(1),     C(16)),    (ELMT(15),   C(30))
      EQUIVALENCE    (DATA(1),     C(31)),    (DATA(23),   C(53))
      EQUIVALENCE    (A(1),        C(421)),   (A(1350),    C(1770))
      EQUIVALENCE    (COEFT(1),    C(421)),   (COEFT(1350),C(1770))
      EQUIVALENCE    (ANS(1),      C(421)),   (ANS(454),   C(874))
      EQUIVALENCE    (HSUM,        C(424)),   (SSUM,       C(425))
      EQUIVALENCE    (WTMOL,       C(426)),   (CP,         C(427))
      EQUIVALENCE    (DLMPT,       C(428)),   (DLMTP,      C(429))
      EQUIVALENCE    (GAMMA,       C(430)),   (ARATIO,     C(431))
      EQUIVALENCE    (VMACH,       C(432)),   (SP IMP,     C(433))
      EQUIVALENCE    (VACI,        C(434)),   (CF,         C(436))
      EQUIVALENCE    (RHOI,        C(437)),   (RHOVAC,     C(438))
      EQUIVALENCE    (RHO,         C(439))
      EQUIVALENCE    (T PI,        C(440)),   (PI I,       C(441))
      EQUIVALENCE    (EP PI,       C(442)),   (AW PI,      C(443))
      EQUIVALENCE    (T ETA,       C(445))
      EQUIVALENCE    (ETA I,       C(446)),   (EP ETA,     C(447))
      EQUIVALENCE    (AW ETA,      C(448)),   (T SIG,      C(450))
      EQUIVALENCE    (SIG I,       C(451)),   (EP SIG,     C(452))
      EQUIVALENCE    (AW SIG,      C(453))
      EQUIVALENCE    (EN(1),       C(1771)),  (EN(90),     C(1860))
      EQUIVALENCE    (BOX(1),      C(1771)),  (BOX(15),    C(1785))
      EQUIVALENCE    (BOF(1),      C(1786)),  (BOF(15),    C(1800))
      EQUIVALENCE    (HX,          C(1801)),  (HF,         C(1802))
      EQUIVALENCE    (VXPLS,       C(1803)),  (VXMIN,      C(1804))
      EQUIVALENCE    (VFPLS,       C(1805)),  (VFMIN,      C(1806))
      EQUIVALENCE    (EN LN(1),    C(1861)),  (EN LN(90),  C(1950))
      EQUIVALENCE    (DEL N(1),    C(1951)),  (DEL N(90),  C(2040))
      EQUIVALENCE    (COEFX(1),    C(1951)),  (COEFX(20),  C(1970))
      EQUIVALENCE    (DX(1),       C(1951)),  (DX(20),     C(1970))
      EQUIVALENCE    (HO(1),       C(2041)),  (HO(90),     C(2130))
      EQUIVALENCE    (S(1),        C(2131)),  (S(90),      C(2220))
      EQUIVALENCE    (X(1),        C(2221)),  (X(20),      C(2240))
      EQUIVALENCE    (FORMLA(1),   C(2221)),  (FORMLA(18),C(2238))
      EQUIVALENCE    (DELTA(1),    C(2241)),  (DELTA(20),  C(2260))
      EQUIVALENCE    (BO(1),       C(2261)),  (BO(15),     C(2275))
      EQUIVALENCE    (PO,          C(2276)),  (HSUBO,      C(2277))
      EQUIVALENCE    (SO,          C(2278)),  (T LN,       C(2279))
      EQUIVALENCE    (T,           C(2280)),  (AAY LN,     C(2281))
      EQUIVALENCE    (AAY,         C(2282)),  (CPSUM,      C(2283))
      EQUIVALENCE    (HC,          C(2284)),  (TC LN,      C(2285))
      EQUIVALENCE    (PCP(1),      C(2286)),  (PCP(25),    C(2310))
      EQUIVALENCE    (PROD(1),     C(2311)),  (PROD(3),    C(2313))
      EQUIVALENCE    (DATUM(1),    C(2311)),  (DATUM(3),   C(2313))
      EQUIVALENCE    (PC,          C(2314)),  (TC,         C(2315))
      EQUIVALENCE    (IPROB,       C(2316)),  (IFIXT,      C(2317))
      EQUIVALENCE    (IHS,         C(2318)),  (ICOND,      C(2319))
      EQUIVALENCE    (ISYM,        C(2320)),  (IPROD,      C(2321))
      EQUIVALENCE    (IDID,        C(2322)),  (LDRUM,      C(2323))
      EQUIVALENCE    (IDRM,        C(2323)),  (KDRUM,      C(2324))
      EQUIVALENCE    (L,           C(2325)),  (L1,         C(2326))
      EQUIVALENCE    (M,           C(2327)),  (M1,         C(2328))
      EQUIVALENCE    (N,           C(2329)),  (IQ,         C(2330))
      EQUIVALENCE    (IQ1,         C(2331)),  (IQ2,        C(2332))

      EQUIVALENCE    (IQ3,         C(2333)),  (KMAT,       C(2334))
      EQUIVALENCE    (IMAT,        C(2335)),  (IUSE,       C(2335))
      EQUIVALENCE    (IADD,        C(2336)),  (ITNUMB,     C(2337))
      EQUIVALENCE    (ITAPE,       C(2338)),  (P,          C(2339))
      EQUIVALENCE    (IDEBUG,      C(2340)),  (IFROZ,      C(2341))
C
      DIMENSION   G(20,21),    A(15,90),    EN(90),      EN LN(90)
      DIMENSION   DEL N(90),   HO(90),      S(90),       X(20)
      DIMENSION   DELTA(20),   BO(15),      PCP(25),     PROD(3)
      DIMENSION   COEFX(20),   DX(20),      FORM(15),    COEFT(15,90)
      DIMENSION   ELMT(15),    DATA(23),    DATUM(3),    FORMLA(18)
      DIMENSION   BOX(15),     BOF(15),     ANS(454),    SYSTM(15)
C
C
S BLK ALF    00000
S RPN ALF    00000)
S LPN ALF    00000(
S GAS AL     00000G
S SOL ALF    00000S
S LIQ ALF    00000L
S PLS ALF    00000+
S MIN ALF    00000-
S E   ALF    00000E
S END ALF    END
S C10 DEC 10
S C12 DEC 12
C
C
      KION=2
      DO 1 K=1,L
S     CLA ELMT(K)
S     SUB E
S     TZE*2
    1 CONTINUE
      GO TO 3
    2 KION=1
S     CLA ELMT(K)
S     LDQ ELMT(L)
S     STQ ELMT(K)
S     STO ELMT(L)
S   3 CLA C10
S     LRS 18
S     STO C10
      ISOL=0
      M=0
      DO 4 J=1,15
      DO 4 K=1,90
    4 COEFT(J,K)=0.0
      DO 5 INT=1,2
    5 WRITE TAPE  I3,   ((COEFT(K,JT),K=1,15),JT=1,90)
      REWIND I3
      WRITE DRUM LDRUM,1,A
    7 READ TAPE ITAPE, (DATA(I),I=1,23)
S     CLA DATA(1)
S     SUB END
S     TZE*171
C
C     UNPACK THE BCD FORMULA FOR THE PRODUCT
C
      DO 16 I=1,2
```

```
    16 DATUM(I)=DATA(I)
       J=1
       I=1
    13 K=0
S   17 SSP
S      CLM
S      LDQ DATUM(I)
S      LGL 6
S      STO FORMLA(J)
S      STQ DATUM(I)
       J=J+1
S      TXH*21,(K),4
       K=K+1
       GO TO 17
S   21 TXH*25,(I),1
       I=I+1
       GO TO 13
C
C      BEGIN SEARCH FOR FIRST NON BLANK ALPHANUMERIC CHARACTER
C
S   25 LXD C12,(J)
S   29 SXD J,(J)
S      CLA FORMLA(J)
S      SUB BLK
S      TNZ*35
S      TIX*29,(J),1
    30 WRITE OUTPUT TAPE 6,31,(DATA(I),I=1,3)
    31 FORMAT (14H THE FORMULA  3A6,33H  IS INCORRECT ON THE MASTER TAPE)
S      TRA*7
S   35 ADD BLK
S      SUB RPN
S      TNZ*30
       J=J-1
S      CLA FORMLA(J)
S      SUB GAS
S      TZE*39
S      ADD GAS
S      SUB SOL
S      TZE*41
S      ADD SOL
S      SUB LIQ
S      TZE*41
S      TRA*30
    39 ITYPE=1
S      TRA*47
    41 ITYPE=2
    47 J=J-1
S      CLA FORMLA(J)
S      SUB LPN
S      TNZ*30
       J=J-1
C
C      OBTAIN AND STORE THE FORMULA NUMBERS A(K,J)
C
       DO 48 K=1,15
    48 FORM(K)=0.0
    51 NLSW=1
       NUMB=0
    55 ICNT=0
    57 JCNT=J-ICNT

       IF (JCNT) 30,81,59
S   59 CLA FORMLA(JCNT)
S      SUB C10
S      TPL*67
       GO TO (63,85),NLSW
    63 ICNT=ICNT+1
       GO TO 57
    67 GO TO (69,63),NLSW
S   69 CLA ICNT
S      TZE*330
       IF (ICNT-2) 77,73,30
   330 IF (KION-1) 30,333,30
   333 NLSW=2
       GO TO 57
S   73 LDQ FORMLA(J-1)
S      MPY C10
S      LLS 18
S      STQ NUMB
S   77 CLA FORMLA(J)
S      LLS 18
S      ADD NUMB
S      STO NUMB
       VALUE=NUMB
       J=J-ICNT
       NLSW=2
       GO TO 55
    81 GO TO (30,85),NLSW
S   85 CLA ICNT
S      TZE*30
S      STZ SYMBL
       IF (NUMB) 86,95,86
    86 IF (ICNT-2) 93,89,30
S   89 LDQ FORMLA(J-1)
S      LLS 41
S      STO SYMBL
S   93 CLA SYMBL
S      ADD FORMLA(J)
S      STO SYMBL
       GO TO 107
    95 IF (JCNT) 30,30,96
S   96 CLA FORMLA(J)
S      SUB PLS
S      TNZ*97
       FORM(L)= -ICNT
       GO TO 109
S   97 ADD PLS
S      SUB MIN
S      TNZ*30
       FORM(L)= ICNT
       GO TO 109
   107 DO 111 K=1,L
S      CLA SYMBL
S      SUB ELMT(K)
S      TZE*105
   111 CONTINUE
       GO TO 7
   105 FORM(K)=VALUE
   109 J=J-ICNT
       IF (J) 30,121,51
   121 IF (ITYPE-1) 30,133,137
```

```
  133 M=M+1
      J=M
      GO TO 141
  137 J=90-ISOL
      ISOL=ISOL+1
  141 READ DRUM LDRUM,1,A
  145 DO 147 K=1,L
      A(K,J)=FORM(K)
  147 CONTINUE
      WRITE DRUM LDRUM,1,A
C
C     WRITE THERMODYNAMIC DATA ON TAPE ORDERED BY INTERVAL
C
  151 IT=0
S     CLA DATA(1)
S     LDQ DATA(3)
S     STO DATA(1)
S     LDQ DATA(2)
S     STO DATA(2)
S     STQ DATA(3)
      DO 163 INT =1,2
      READ TAPE I3, ((COEFT(K,JT),K=1,15),JT=1,90)
      DO 155 K=1,5
      COEFT(K,J)=DATA(K)
  155 CONTINUE
      DO 159 K=6,14
      KIT= K+IT
      COEFT(K,J)=DATA(KIT)
  159 CONTINUE
      IT=IT+9
      WRITE TAPE I4, ((COEFT(K,JT),K=1,15),JT=1,90)
  163 CONTINUE
      REWIND I3
      REWIND I4
S     CLA I3
S     LDQ I4
S     STO I4
S     STQ I3
      GO TO 7
C
C     GO TO NEXT MOLECULE
C
C
C     ELIMINATE GAP BETWEEN GASES AND CONDENSED PHASES
C
  171 N=M+ISOL
      JEER=1
  173 IF (N-90) 175,224,181
  175 IF (ISOL) 177,224,184
  177 JEER=2
      GO TO 224
  181 WRITE OUTPUT TAPE 6,182
  182 FORMAT (45H TOO MANY REACTION PRODUCTS FOUND ON THE TAPE)
      JEER=2
      GO TO 224
  184 DO 187 I=1,2
      READ TAPE I3, ((COEFT(K,JT),K=1,15),JT=1,90)
      KK=90-ISOL
      DO  186 J=1,ISOL
      MJ=M+J

      KJ=KK+J
      DO  185 K=1,15
      COEFT(K,MJ)=COEFT(K,KJ)
  185 CONTINUE
  186 CONTINUE
      WRITE TAPE I4, ((COEFT(K,JT),K=1,15),JT=1,90)
  187 CONTINUE
      REWIND I3
      REWIND I4
  215 READ DRUM LDRUM,1,A
      DO 219 J=1,ISOL
      MJ=M+J
      KJ=KK+J
      DO 217 K=1,15
      A(K,MJ)=A(K,KJ)
  217 CONTINUE
  219 CONTINUE
      WRITE DRUM LDRUM,1,A
      GO TO 225
S 224 CLA I3
S     LDQ I4
S     STO I4
S     STQ I3
  225 RETURN
```

```
      SUBROUTINE BYPASS (J,IARG)
C
C
      COMMON C
      EQUIVALENCE   (G(1),      C(1)),      (G(420),    C(420))
      EQUIVALENCE   (FORM(1),   C(1)),      (FORM(15),  C(15))
      EQUIVALENCE   (ELMT(1),   C(16)),     (ELMT(15),  C(30))
      EQUIVALENCE   (DATA(1),   C(31)),     (DATA(23),  C(53))
      EQUIVALENCE   (A(1),      C(421)),    (A(1350),   C(1770))
      EQUIVALENCE   (COEFT(1),  C(421)),    (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),    C(421)),    (ANS(454),  C(874))
      EQUIVALENCE   (HSUM,      C(424)),    (SSUM,      C(425))
      EQUIVALENCE   (WTMOL,     C(426)),    (CP,        C(427))
      EQUIVALENCE   (DLMPT,     C(428)),    (DLMTP,     C(429))
      EQUIVALENCE   (GAMMA,     C(430)),    (ARATIO,    C(431))
      EQUIVALENCE   (VMACH,     C(432)),    (SP IMP,    C(433))
      EQUIVALENCE   (VACI,      C(434)),    (CF,        C(436))
      EQUIVALENCE   (RHOI,      C(437)),    (RHOVAC,    C(438))
      EQUIVALENCE   (RHO,       C(439))
      EQUIVALENCE   (T PI,      C(440)),    (PI I,      C(441))
      EQUIVALENCE   (EP PI,     C(442)),    (AW PI,     C(443))
      EQUIVALENCE   (T ETA,     C(445))
      EQUIVALENCE   (ETA I,     C(446)),    (EP ETA,    C(447))
      EQUIVALENCE   (AW ETA,    C(448)),    (T SIG,     C(450))
      EQUIVALENCE   (SIG I,     C(451)),    (EP SIG,    C(452))
      EQUIVALENCE   (AW SIG,    C(453))
      EQUIVALENCE   (EN(1),     C(1771)),   (EN(90),    C(1860))
      EQUIVALENCE   (BOX(1),    C(1771)),   (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),    C(1786)),   (BOF(15),   C(1800))
      EQUIVALENCE   (HX,        C(1801)),   (HF,        C(1802))
      EQUIVALENCE   (VXPLS,     C(1803)),   (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,     C(1805)),   (VFMIN,     C(1806))
      EQUIVALENCE   (EN LN(1),  C(1861)),   (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),  C(1951)),   (DEL N(90), C(2040))
      EQUIVALENCE   (COEFX(1),  C(1951)),   (COEFX(20), C(1970))
      EQUIVALENCE   (DX(1),     C(1951)),   (DX(20),    C(1970))
      EQUIVALENCE   (HO(1),     C(2041)),   (HO(90),    C(2130))
      EQUIVALENCE   (S(1),      C(2131)),   (S(90),     C(2220))
      EQUIVALENCE   (X(1),      C(2221)),   (X(20),     C(2240))
      EQUIVALENCE   (FORMLA(1), C(2221)),   (FORMLA(18),C(2238))
      EQUIVALENCE   (DELTA(1),  C(2241)),   (DELTA(20), C(2260))
      EQUIVALENCE   (BO(1),     C(2261)),   (BO(15),    C(2275))
      EQUIVALENCE   (PO,        C(2276)),   (HSUBO,     C(2277))
      EQUIVALENCE   (SO,        C(2278)),   (T LN,      C(2279))
      EQUIVALENCE   (T,         C(2280)),   (AAY LN,    C(2281))
      EQUIVALENCE   (AAY,       C(2282)),   (CPSUM,     C(2283))
      EQUIVALENCE   (HC,        C(2284)),   (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),    C(2286)),   (PCP(25),   C(2310))
      EQUIVALENCE   (PROD(1),   C(2311)),   (PROD(3),   C(2313))
      EQUIVALENCE   (DATUM(1),  C(2311)),   (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,        C(2314)),   (TC,        C(2315))
      EQUIVALENCE   (IPROB,     C(2316)),   (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,       C(2318)),   (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,      C(2320)),   (IPROD,     C(2321))
      EQUIVALENCE   (IDID,      C(2322)),   (LDRUM,     C(2323))
      EQUIVALENCE   (IDRM,      C(2323)),   (KDRUM,     C(2324))
      EQUIVALENCE   (L,         C(2325)),   (L1,        C(2326))
      EQUIVALENCE   (M,         C(2327)),   (M1,        C(2328))
      EQUIVALENCE   (N,         C(2329)),   (IQ,        C(2330))
      EQUIVALENCE   (IQ1,       C(2331)),   (IQ2,       C(2332))

      EQUIVALENCE   (IQ3,       C(2333)),   (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,      C(2335)),   (IUSE,      C(2335))
      EQUIVALENCE   (IADD,      C(2336)),   (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,     C(2338)),   (P,         C(2339))
      EQUIVALENCE   (IDEBUG,    C(2340)),   (IFROZ,     C(2341))
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15),   COEFT(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),.   BOF(15),    ANS(454),   SYSTM(15)
C
C
C     IARG=1 MEANS TEST ONLY, IARG=2 MEANS ELIMINATE A SPECIES, IARG=3
C     MEANS ADD ANOTHER SPECIES
C
S     LXD J,(J)
S     TXL*2,(J),35
S     TXL*1,(J),70
      K=3
S     TIX*3,(J),70
    1 K=2
S     TIX*3,(J),35
    2 K=1
    3 IF (IARG-2) 4,5,7
    4 IPROD=2
S     CLA PROD(K)
S     LRS 35,(J)
S     LBT
S     TRA*10
      IPROD=1
S     TRA*10
S   5 CLA PROD(K)
S     LRS 35,(J)
S     LBT
S     TRA*6
S     TRA*10
S   6 COM
S     LRS 1
S     COM
S     LLS 36,(J)
S     STO PROD(K)
S     CLA M
S     SUB J
S     TPL*10
      IQ3=IQ2
      IQ2=IQ1
      IQ1=IQ
      IQ =IQ-1
S     TRA*9
S   7 CLA PROD (K)
S     LRS 35,(J)
S     LBT
S     TRA*10
S     COM
S     LRS 1
S     COM
S     LLS 36,(J)
S     STO PROD(K)

S     CLA M
S     SUB J
S     TPL*10
      IQ =IQ1
      IQ1=IQ2
      IQ2=IQ3
      IQ3=IQ3+1
    9 SENSE LIGHT 4
   10 RETURN
```

```
      SUBROUTINE INPUT
C
C
      COMMON C
      EQUIVALENCE(ATOM(1),C(1111)),(ATOM(303),C(1413))
      EQUIVALENCE   (G(1),       C(1)),     (G(420),    C(420))
      EQUIVALENCE   (FORM(1),    C(1)),     (FORM(15),  C(15))
      EQUIVALENCE   (ELMT(1),    C(16)),    (ELMT(15),  C(30))
      EQUIVALENCE   (DATA(1),    C(31)),    (DATA(23),  C(53))
      EQUIVALENCE   (A(1),       C(421)),   (A( 690),   C(1110))
      EQUIVALENCE   (COEFT(1),   C(421)),   (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),     C(421)),   (ANS(454),  C(874))
      EQUIVALENCE   (HSUM,       C(424)),   (SSUM,      C(425))
      EQUIVALENCE   (WTMOL,      C(426)),   (CP,        C(427))
      EQUIVALENCE   (DLMPT,      C(428)),   (DLMTP,     C(429))
      EQUIVALENCE   (GAMMA,      C(430)),   (ARATIO,    C(431))
      EQUIVALENCE   (VMACH,      C(432)),   (SP IMP,    C(433))
      EQUIVALENCE   (VACI,       C(434)),   (CF,        C(436))
      EQUIVALENCE   (RHOI,       C(437)),   (RHOVAC,    C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),   (PI I,      C(441))
      EQUIVALENCE   (EP PI,      C(442)),   (AW PI,     C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),   (EP ETA,    C(447))
      EQUIVALENCE   (AW ETA,     C(448)),   (T SIG,     C(450))
      EQUIVALENCE   (SIG I,      C(451)),   (EP SIG,    C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQUIVALENCE   (EN(1),      C(1771)),  (EN(90),    C(1860))
      EQUIVALENCE   (BOX(1),     C(1771)),  (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)),  (BOF(15),   C(1800))
      EQUIVALENCE   (HX,         C(1801)),  (HF,        C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)),  (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)),  (VFMIN,     C(1806))
      EQUIVALENCE   (EN LN(1),   C(1861)),  (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)),  (DEL N(90), C(2040))
      EQUIVALENCE   (COEFX(1),   C(1951)),  (COEFX(20), C(1970))
      EQUIVALENCE   (DX(1),      C(1951)),  (DX(20),    C(1970))
      EQUIVALENCE   (HO(1),      C(2041)),  (HO(90),    C(2130))
      EQUIVALENCE   (S(1),       C(2131)),  (S(90),     C(2220))
      EQUIVALENCE   (X(1),       C(2221)),  (X(20),     C(2240))
      EQUIVALENCE   (FORMLA(1),  C(2221)),  (FORMLA(18),C(2238))
      EQUIVALENCE   (DELTA(1),   C(2241)),  (DELTA(20), C(2260))
      EQUIVALENCE   (BO(1),      C(2261)),  (BO(15),    C(2275))
      EQUIVALENCE   (PO,         C(2276)),  (HSUBO,     C(2277))
      EQUIVALENCE   (SO,         C(2278)),  (T LN,      C(2279))
      EQUIVALENCE   (T,          C(2280)),  (AAY LN,    C(2281))
      EQUIVALENCE   (AAY,        C(2282)),  (CPSUM,     C(2283))
      EQUIVALENCE   (HC,         C(2284)),  (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)),  (PCP(25),   C(2310))
      EQUIVALENCE   (PROD(1),    C(2311)),  (PROD(3),   C(2313))
      EQUIVALENCE   (DATUM(1),   C(2311)),  (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,         C(2314)),  (TC,        C(2315))
      EQUIVALENCE   (IPROB,      C(2316)),  (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,        C(2318)),  (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,       C(2320)),  (IPROD,     C(2321))
      EQUIVALENCE   (IDID,       C(2322)),  (LDRUM,     C(2323))
      EQUIVALENCE   (IDRM,       C(2323)),  (KDRUM,     C(2324))
      EQUIVALENCE   (L,          C(2325)),  (L1,        C(2326))
      EQUIVALENCE   (M,          C(2327)),  (M1,        C(2328))
      EQUIVALENCE   (N,          C(2329)),  (IQ,        C(2330))

      EQUIVALENCE   (IQ1,        C(2331)),  (IQ2,       C(2332))
      EQUIVALENCE   (IQ3,        C(2333)),  (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,       C(2335)),  (IUSE,      C(2335))
      EQUIVALENCE   (IADD,       C(2336)),  (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)),  (P,         C(2339))
      EQUIVALENCE   (IDEBUG,     C(2340)),  (IFROZ,     C(2341))
C
      DIMENSION   G(20,21),                 EN(90),     EN LN(90)
      DIMENSION   DEL N(90),   HO(90),      S(90),      X(20)
      DIMENSION   DELTA(20),   BO(15),      PCP(25),    PROD(3)
      DIMENSION   COEFX(20),   DX(20),      FORM(15),   COEFT(15,90)
      DIMENSION   ELMT(15),    DATA(23),    DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),     BOF(15),     ANS(454),   SYSTM(15)
      DIMENSION A(15,46),ATOM(101,3),ANAME(5),ANUM(5)
C
C
C   SUBROUTINE TO COMPUTE PROPELLANTS
C
SOX   ALF   O
      READ DRUM 4,485,JEAN,ATOM
      IF(JEAN-222)51,50,51
   51 CALL BCREAD(ATOM(101,3),ATOM(1,1))
   50 DO 52 I=1,15
S     STZ ELMT(I)
S     STZ BOX(I)
S     STZ BOF(I)
      DO 52 J=1,46
S  52 STZ A(I,J)
S     STZ TOTAL
      NF=0
      NO=0
      NE=0
      WRITE OUTPUT TAPE 6,400
  400 FORMAT(8H1  INPUT//)
  100 READ INPUT TAPE 7,1,(ANAME(I),ANUM(I),I=1,5),PECWT,ENTH,
     2DEN,TEMP,ETHR,DENS
    1 FORMAT(5(A2,F7.5),F8.5,F9.5,A1,F8.5,A1,F8.5)
      IF(ANUM(1))99,200,99
   99 WRITE OUTPUT TAPE 6,402,(ANAME(I),ANUM(I),I=1,5),PECWT,ENTH,DEN,
     2TEMP,ETHR,DENS
  402 FORMAT (1X,5(A2,1X,F7.4,2X),F8.4,2X,F9.2,2X,A1,2X,F8.3,2X,
     2A1,3X,F8.5)
      DO 9 I=1,5
    9 TOTAL=TOTAL+ANUM(I)
      IF(ETHR-OX)11,10,11
   10 NO=NO+1
      KK=NO
      KKK=NO
      NN=31
      GO TO 12
   11 NF=NF+1
      KK=NF+15
      KKK=NF
      NN=32
   12 DO 98 J=1,5
      IF(ANUM(J)) 96,97,96
   96 DO 31 I=1,15
      IF(ANAME(J)-ELMT(I)) 21,20,21
   20 NHUT=0
   33 KT=I
```

```
      GO TO 30
   21 IF(ELMT(I)) 31,22,31
   22 ELMT(I)=ANAME(J)
      NE=NE+1
      NHUT=1
      GO TO 33
   31 CONTINUE
   30 IF(NHUT)14,15,14
   14 DO 16 I=1,101
S     CLA ATOM(I,1)
S     SUB ANAME(J)
S     TNZ*16
   17 II=I
      GO TO 18
   16 CONTINUE
      WRITE OUTPUT TAPE 6,199
  199 FORMAT (32H0 THERE IS A BAD PROPELLANT CARD)
      L=-1
      RETURN
   18 A(NE,37)=ATOM(II,2)
      A(NE,38)=ATOM(II,3)
   15 A(KT,KK)=ANUM(J)
   98 CONTINUE
   97 A(KKK,NN)=ENTH
      A(KKK,NN+2)=PECWT
      A(KKK,NN+4)=DENS
      A(KKK,NN+10)=DEN
      A(KKK,NN+12)=TEMP
      A(KKK,NN+14)=ETHR
      GO TO 100
  200 IF(NE)202,201,202
  201 L=0
      RETURN
  202 JEAN=222
S     STZ WX
S     STZ WF
S     STZ HX
S     STZ HF
S     STZ RHOX
S     STZ RHOF
S     STZ VXPLS
S     STZ VXMIN
S     STZ VFPLS
S     STZ VFMIN
      DO552 J=1,NO
      DO552 I=1,NE
  552 A(J,39)=A(J,39)+A(I ,37)*A(I ,J )
      DO 53 J=1,NF
      DO 53 I=1,NE
   53 A(J,40)=A(J,40)+A(I,37)*A(I,J+15)
      DO550 I=1,NO
   54 HX=HX+A(I,31)*A(I,33)/A(I,39)
  550 WX=WX+A(I,33)
      DO551 I=1,NF
   55 HF=HF+A(I,32)*A(I,34)/A(I,40)
  551 WF=WF+A(I,34)
S     STZ ACX
S     STZ ACF
S     STZ AMX
S     STZ AMF

      DO 42 I=1,NO
      ACX=ACX+A(I,35)*A(I,33)/A(I,39)
   42 AMX=AMX+A(I,33)/A(I,39)
      ACX=ACX/WX
      AMX=WX/AMX
      DO 43 I=1,NF
      ACF=ACF+A(I,36)*A(I,34)/A(I,40)
   43 AMF=AMF+A(I,34)/A(I,40)
      ACF=ACF/WF
      AMF=WF/AMF
      WRITE DRUM 4,1516,ACX,ACF,AMX,AMF
      HX=HX/WX
      HF=HF/WF
      DO 60 I=1,NO
      IF(A(I,35))60,71,60
   60 RHOX=RHOX+A(I,33)/A(I,35)
      RHOX=WX/RHOX
   73 DO 61 I=1,NF
      IF(A(I,36))61,71,61
   61 RHOF=RHOF+A(I,34)/A(I,36)
      RHOF=WF/RHOF
      GO TO 74
S  71 STZ RHOX
S  72 STZ RHOF
   74 DO 57 I=1,NE
      DO 56 J=1,NO
   56 BOX(I)=BOX(I)+A(I,J)*A(J,33)/A(J,39)
   57 BOX(I)=BOX(I)/WX
      DO 59 I=1,NE
      DO 58 J=1,NF
   58 BOF(I)=BOF(I)+A(I,J+15)*A(J,34)/A(J,40)
   59 BOF(I)=BOF(I)/WF
      DO 62 I=1,NE
      IF(A(I,38))63,62,64
   64 VXPLS=VXPLS+BOX(I)*A(I,38)
   67 VFPLS=VFPLS+BOF(I)*A(I,38)
      GO TO 62
   63 VXMIN=VXMIN+BOX(I)*A(I,38)
   66 VFMIN=VFMIN+BOF(I)*A(I,38)
   62 CONTINUE
      WRITE DRUM LDRUM,1996,BOX,BOF,HX,VXPLS,VXMIN,HF,VFPLS,VFMIN
     2,RHOX,RHOF
      DO 40 I=1,NO
   40 A(I,33)=A(I,33)/WX
      DO 41 I=1,NF
   41 A(I,34)=A(I,34)/WF
      TOTAL = MODF(TOTAL,1.0)
      IF(TOTAL)1142,1143,1142
 1142 KD=1
      GO TO 1144
 1143 KD=0
 1144 WRITE DRUM 4,485,JEAN,ATOM
      WRITE DRUM 4,795,A,NF,NO,NE,ELMT,KD
      L=NE
      RETURN
```

```
C     MAIN PROGRAM TWO
C
      COMMON C
      EQUIVALENCE   (G(1),       C(1)),     (G(420),     C(420))
      EQUIVALENCE   (FORM(1),    C(1)),     (FORM(15),   C(15))
      EQUIVALENCE   (ELMT(1),    C(16)),    (ELMT(15),   C(30))
      EQUIVALENCE   (DATA(1),    C(31)),    (DATA(23),   C(53))
      EQUIVALENCE   (A(1),       C(421)),   (A(1350),    C(1770))
      EQUIVALENCE   (COEFT(1),   C(421)),   (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),     C(421)),   (ANS(454),   C(874))
      EQUIVALENCE   (HSUM,       C(424)),   (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,      C(426)),   (CP,         C(427))
      EQUIVALENCE   (DLMPT,      C(428)),   (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,      C(430)),   (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,      C(432)),   (SP IMP,     C(433))
      EQUIVALENCE   (VACI,       C(434)),   (CF,         C(436))
      EQUIVALENCE   (RHOI,       C(437)),   (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),   (PI I,       C(441))
      EQUIVALENCE   (EP PI,      C(442)),   (AW PI,      C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),   (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,     C(448)),   (T SIG,      C(450))
      EQUIVALENCE   (SIG I,      C(451)),   (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQUIVALENCE   (EN(1),      C(1771)),  (EN(90),     C(1860))
      EQUIVALENCE   (BOX(1),     C(1771)),  (BOX(15),    C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)),  (BOF(15),    C(1800))
      EQUIVALENCE   (HX,         C(1801)),  (HF,         C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)),  (VXMIN,      C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)),  (VFMIN,      C(1806))
      EQUIVALENCE   (EN LN(1),   C(1861)),  (EN LN(90),  C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)),  (DEL N(90),  C(2040))
      EQUIVALENCE   (COEFX(1),   C(1951)),  (COEFX(20),  C(1970))
      EQUIVALENCE   (DX(1),      C(1951)),  (DX(20),     C(1970))
      EQUIVALENCE   (HO(1),      C(2041)),  (HO(90),     C(2130))
      EQUIVALENCE   (S(1),       C(2131)),  (S(90),      C(2220))
      EQUIVALENCE   (X(1),       C(2221)),  (X(20),      C(2240))
      EQUIVALENCE   (FORMLA(1),  C(2221)),  (FORMLA(18), C(2238))
      EQUIVALENCE   (DELTA(1),   C(2241)),  (DELTA(20),  C(2260))
      EQUIVALENCE   (BO(1),      C(2261)),  (BO(15),     C(2275))
      EQUIVALENCE   (PO,         C(2276)),  (HSUBO,      C(2277))
      EQUIVALENCE   (SO,         C(2278)),  (T LN,       C(2279))
      EQUIVALENCE   (T,          C(2280)),  (AAY LN,     C(2281))
      EQUIVALENCE   (AAY,        C(2282)),  (CPSUM,      C(2283))
      EQUIVALENCE   (HC,         C(2284)),  (TC LN,      C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)),  (PCP(25),    C(2310))
      EQUIVALENCE   (PROD(1),    C(2311)),  (PROD(3),    C(2313))
      EQUIVALENCE   (DATUM(1),   C(2311)),  (DATUM(3),   C(2313))
      EQUIVALENCE   (PC,         C(2314)),  (TC,         C(2315))
      EQUIVALENCE   (IPROB,      C(2316)),  (IFIXT,      C(2317))
      EQUIVALENCE   (IHS,        C(2318)),  (ICOND,      C(2319))
      EQUIVALENCE   (ISYM,       C(2320)),  (IPROD,      C(2321))
      EQUIVALENCE   (IDID,       C(2322)),  (LDRUM,      C(2323))
      EQUIVALENCE   (IDRM,       C(2323)),  (KDRUM,      C(2324))
      EQUIVALENCE   (L,          C(2325)),  (L1,         C(2326))
      EQUIVALENCE   (M,          C(2327)),  (M1,         C(2328))
      EQUIVALENCE   (N,          C(2329)),  (IQ,         C(2330))
      EQUIVALENCE   (IQ1,        C(2331)),  (IQ2,        C(2332))
      EQUIVALENCE   (IQ3,        C(2333)),  (KMAT,       C(2334))

      EQUIVALENCE   (IMAT,       C(2335)),  (IUSE,       C(2335))
      EQUIVALENCE   (IADD,       C(2336)),  (ITNUMB,     C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)),  (P,          C(2339))
      EQUIVALENCE   (IDEBUG,     C(2340)),  (IFROZ,      C(2341))
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15),   COEFT(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
C
S MT  ALF
S GAS ALF   00000G
S BLK ALF   00000
C
      REWIND 3
      NO EQ=0
      ITEST=M1
      SIZE=18.5
  555 IF (IPROB-3) 557,563,565
  557 PC=PC/14.696006
      PO=PC
      IF (TC) 559,559,561
  559 TC LN= 8.25
      GO TO 431
  561 TC LN=LOGF(TC)
      GO TO 431
  563 PO=PC
      GO TO 431
  565 T=TC
      PO=0.0
      T LN=LOGF(T)
C
C     START CALCULATION FOR NEW OVERALL COMPOSITION
C
  431 IADD=1
      IF (IFROZ)  1431,379,1432
 1431 READ DRUM 4,479,IUSE
      IF (IUSE) 1432,1432,433
 1432 DO 432 K=1,N
      EN(K)=0.0
      EN LN(K)=0.0
  432 DEL N(K)=0.0
      AAY LN=5.0
  433 SENSE LIGHT 0
      IF (IPROB-2) 435,445,434
  434 IF (IPROB-4) 455,465,379
  435 IF (IADD-1) 379,436,441
  436 SENSE LIGHT 1
  437 T LN=TC LN
      ITROT=3
  438 IF (PCP(IADD)) 231,231,439
  439 SENSE LIGHT 4
      PO=PC/PCP(IADD)
      GO TO 13
  441 IF (IADD-25) 438,438,231
  445 IF (IADD-1) 379,447,441
  447 SENSE LIGHT 2
      GO TO 437
```

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  455 IF (IADD-25) 459,459,231
  459 IF (PCP(IADD)) 231,231,460
  460 T=PCP(IADD)
      T LN= LOGF(T)
      GO TO 473
  465 IF (IADD-25) 469,469,231
  469 IF (PCP(IADD)) 231,231,470
  470 PO=PCP(IADD)
  473 SENSE LIGHT 2
      SENSE LIGHT 4
C
C     BEGIN CALCULATIONS FOR CURRENT POINT
C     CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
C
   13 READ DRUM KDRUM,1,COEFT
      PO LN=LOGF(PO)
      IF (IPROB-2) 17,17,19
   17 T=EXPF(T LN)
   19 IF (COEFT(7,1)-T) 21,27,27
   21 IF (COEFT(7,1)-5000.0) 23,31,231
   23 BACKSPACE ITAPE
      BACKSPACE ITAPE
   25 READ TAPE ITAPE, ((COEFT(K,J),K=1,15),J=1,90)
      WRITE DRUM KDRUM,1,COEFT
      SENSE LIGHT 4
      GO TO 19
   27 IF (T-COEFT(6,1)) 29,37,37
   29 IF (300.0-COEFT(6,1)) 25,31,231
   31 IF (SENSE LIGHT 4) 38,305
C
C     ELIMINATE THOSE SPECIES WHICH DO NOT HAVE DATA IN THIS INTERVAL
C
   37 IF (SENSE LIGHT 4 ) 38,142
   38 SENSE LIGHT 4
      DO 40 J=1,N
      IF (COEFT(8,J)) 40,39,4
   39 CALL BYPASS (J,2)
      EN LN(J)=0.0
      EN(J)=0.0
   40 CONTINUE
C
C     BEGIN ITERATION FOR COMPOSITION
C
   42 IQ=IO
      IQ1=IQ1
      IQ2=IQ2
      IQ3=IQ3
      ITNUMB=30
   43 DO 48 J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 48,45,48
   45 IF (EN LN(J)+SIZE-PO LN) 46,46,47
   46 EN(J)=0.0
      GO TO 48
   47 EN(J)=EXPF(EN LN(J))
   48 CONTINUE
      IF (IPROB-2) 49,49,51
   49 T=EXPF(T LN)
   51 AAY=EXPF(AAY LN)
      READ DRUM KDRUM,1,COEFT

C
C     CALCULATE HEAT CAPACITY, ENTHALPY AND ENTROPY
C
      IFIXT=3
      IF (SENSE LIGHT 2) 52,55
   52 SENSE LIGHT 2
      IF (SENSE LIGHT 4) 53,55
   53 SENSE LIGHT 4
      IFIXT=1
      IF (ITNUMB-30) 55,54,55
   54 IFIXT=2
   55 CPSUM=0.0
      DO 60 J=1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 60,56,60
   56 IF (IFIXT-2) 59,58,57
   57 CPSUM=CPSUM+((((COEFT(12,J)*T+COEFT(11,J))*T+COEFT(10,J))*T+COEFT(
     19,J))*T+COEFT(8,J))*EN(J)
   58 HO(J)=((((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
     1+COEFT(9,J)/2.0)*T +COEFT(13,J)/T+COEFT(8,J)
   59 S(J)=((((COEFT(12,J)/4.0 )*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
     1+COEFT(9,J))*T+COEFT(8,J)*T LN+COEFT(14,J)-EN LN(J)
   60 CONTINUE
C
C     CONSTRUCT MATRIX AND SOLVE THE EQUATIONS
C
      READ DRUM LDRUM,1,A
      CALL MATRIX
      IF (SENSE LIGHT 4) 61,171
   61 SENSE LIGHT 4
      CALL GAUSS (1576)
      IF (IDEBUG) 910,80,910
  910 DO 911 I=1,IMAT
  911 WRITE OUTPUT TAPE 6,912,(G(I,K),K=1,KMAT),DELTA(I)
      WRITE OUTPUT TAPE 6,912,(X(I),I=1,IMAT)
  912 FORMAT (8E14.6)
   80 IF (IDID-IMAT) 81,85,81
   81 IF (SIZE-18.5) 83,83,311
   83 SIZE=27.5
      GO TO 43
   85 ITNUMB=ITNUMB-1
      DO 87 K=1,IMAT
      IF (ABSF(DELTA(K))-0.5E-4) 87,87,315
   87 CONTINUE
C
C     OBTAIN CORRECTIONS TO THE ESTIMATES
C
      D LN T=X(IQ2)
   91 IF (IFIXT-2) 93,95,379
   93 D LN T=0.0
   95 DO  101 J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 96,97,96
   96 DEL N(J)=0.0
      GO TO 101
   97 DEL N(J)=HO(J)*D LN T-HO(J)+S(J)
      DO  99 K=1,L
   99 DEL N(J)=DEL N(J)+A(K,J)*X(K)
  101 CONTINUE
      IF (L-IQ) 103,109,109
```

```
  103 J=M1
      DO 107 K=L1,IO
  104 CALL BYPASS (J,1)
      IF (IPROD-2) 105,106,105
  105 DEL N(J)=0.0
      J=J+1
      GO TO 104
  106 DEL N(J)=X(K)
      J=J+1
  107 CONTINUE
  109 AMBDA=1.0
      AMBDA1=1.0
S     CLA D LN T
S     SSP
S     SBM X(IQ1)
S     TPL*913
      SUM=ABSF(X(IQ1))
      GO TO 915
  913 SUM=ABSF(D LN T)
  915 DO 917 J=1,M
      IF (EN(J)) 917,1915,916
  916 SUM=MAX1F(DEL N(J),SUM)
      GO TO 917
 1915 IF (DEL N(J)) 917,917,1917
 1917 SUM1=ABSF((P0 LN-9.212-EN LN(J))/DEL N(J))
      AMBDA1=MIN1F(SUM1,AMBDA1)
  917 CONTINUE
      IF (SUM-2.0) 1110,1110,110
  110 AMBDA=2.0/SUM
 1110 AMBDA=MIN1F(AMBDA,AMBDA1)
  920 IF (IDEBUG) 921,111,921
  921 READ DRUM KDRUM,1,COEFT
      WRITE OUTPUT TAPE 6,923, T,P,AAY, AMBDA, ((COEFT(K,J),K=1,3),
     1  EN(J),EN LN(J),DEL N(J),H0(J),S(J),J=1,N)
  923 FORMAT (4E25.8/(1X,3A6,5E15.6))
C
C     APPLY CORRECTIONS TO THE ESTIMATES
C
  111 DO 113 J=1,M
  113 EN LN(J)=EN LN(J)+AMBDA*DEL N(J)
      IF (ICOND-2) 115,121,375
  115 DO 117 J=M1,N
  117 EN(J)=EN(J)+AMBDA*DEL N(J)
  121 T LN=T LN +AMBDA*D LN T
      AAY LN=AAY LN- AMBDA*X(IQ1)
      IF (SENSE SWITCH 6) 122,124
  122 IF (IDEBUG) 1122,123,1122
 1122 IDEBUG=0                                    - see errata
      GO TO 231
  123 IDEBUG=1
C
C     TEST  FOR CONVERGENCE OF ITERATION
C
  124 IF (ITNUMB) 125,132,125
  125 IF (AMBDA-1.0) 43,1124,231
 1124 P=0.0
      DO 1126 J=1,M
 1126 P=P+EXPF(EN LN(J))
      IF (ABSF((P0-P)/P0)-0.5E-5) 126,126,43
  126 SUM=P

      IF(ICOND-2)127,129,375
  127 DO 128 J=M1,N
  128 SUM=SUM+ABSF(EN(J))
  129 DO 130 J=1,N
      IF (J-M) 1129,1129,1130
 1129 IF (ABSF(EN(J)*DEL N(J)/SUM)-0.5E-5) 130,130,43
 1130 IF (ABSF(DEL N(J)/SUM)-0.5E-5) 130,130,43
  130 CONTINUE
  132 IF (SENSE LIGHT 4) 133,133
  133 GO TO 13
C
C     ELIMINATE THOSE SPECIES WITH NO DATA AT THIS TEMPERATURE, ADD
C     THOSE WITH DATA AT THIS TEMPERATURE
C
  142 DO 170 J=1,N
S     CLA COFFT(1,J)
S     SUB MT
S     TNZ*170
      IF (COEFT(5,J)+100.0-T) 285,143,143
  143 IF (T-COEFT(4,J)+100.0) 295,144,144
  285 IF (5000.0-COEFT(5,J)) 144,144,301
  295 IF (COEFT(4,J)-300.0) 144,144,301
  144 IF (J-M) 145,145,146
  145 CALL BYPASS (J,3)
      GO TO 170
  301 CALL BYPASS (J,2)
      EN(J)=0.0
      EN LN(J)=0.0
      DEL N(J)=0.0
      GO TO 170
  146 IF (EN(J)) 147,148,170
  147 EN(J)=0.0
      DEL N(J)=0.0
      CALL BYPASS (J,2)
      GO TO 42
C
C     SKIP CONDENSATION CHECK IF T IS HIGHER THAN MELTING POINT WHEN
C     TESTING SOLID, OR LOWER THAN MELTING POINT WHEN TESTING LIQUID
C
  148 IF (COEFT(4,J)-COEFT(5,J-1)) 150,149,150
  149 IF (COEFT(4,J)-T) 153,153,170
  150 IF (COEFT(5,J)-COEFT(4,J+1)) 153,151,153
  151 IF (T-COEFT(5,J)) 153,153,170
C
C     CHECK FOR CONDENSATION
C     IF MORE THAN ONE CONDENSED PHASE OF ANY SPECIES CAN EXIST THE
C     PHASE STABLE AT THE HIGHER TEMPERATURE MUST PRECEED THAT STABLE AT
C     THE LOWER TEMPERATURE ON MASTER TAPE
C
  153 DO 155 K=2,3
      SUM=COEFT(K,J)
      DO 154 I=1,6
S     LDQ SUM
S     CLM
S     SSP
S     LGL 6
S     STQ SUM
S     SUB BLK
S     TZE*156
  154 CONTINUE
```

```
   155 CONTINUE
       K=3
       I=5
       GO TO 159
   156 I=I-2
       IF (I) 157,158,159
   157 K=2
       I=5
       GO TO 159
   158 K=2
       I=6
   159 FORM(2)=COEFT(2,J)
       FORM(3)=COEFT(3,J)
       I=6*I
       JJ=42-I
S      LXD I,(I)
S      LXD JJ,(JJ)
S      LDQ FORM(K)
S      CLM
S      SSP
S      LGL 36,(JJ)
S      SLW SUM
S      LGL 6
S      CLM
S      ADD GAS
S      LGL 36,(I)
S      SLW SUM1
S      LDQ SUM1
S      LGL 36,(JJ)
S      CAL SUM
S      LGL 42,(I)
S      SLW FORM(K)
       DO 160 K=1,M
S      CLA FORM(2)
S      SUB COEFT(2,K)
S      TNZ*160
S      CLA FORM(3)
S      SUB COEFT(3,K)
S      TZE*162
   160 CONTINUE
       CALL BYPASS (J,3)
       GO TO 170
   162 CALL BYPASS (K,1)
       IF (IPROD-2) 170,163,17
   163 HO(J)=((((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
      1+COEFT(9,J)/2.0)*T +COEFT(13,J)/T+COEFT(8,J)
       S(J)=((((COEFT(12,J)/4.0 )*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
      1+COEFT(9,J))*T+COEFT(8,J)*T LN+COEFT(14,J)
       IF (HO(J)-S(J)-HO(K)+S(K)) 164,164,170
   164 CALL BYPASS (J,3)
       EN(J)=0.0
       GO TO 42
   170 CONTINUE
C
C      IF COMPOSITION HAS BEEN CORRECTLY DETERMINED CALCULATE THE
C      EQUILIBRIUM PROPERTIES, OTHERWISE CONTINUE ITERATION
C
       IF (SENSE LIGHT 4) 1171,1172
  1171 SENSE LIGHT 4
       GO TO 42


  1172 IF (ITNUMB) 42,971,42
   971 WRITE OUTPUT TAPE 6,973,IADD
   973 FORMAT (70HL30 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS
      1 FOR THE POINT I5)
       GO TO 42
C
C      CALCULATE EQUILIBRIUM PROPERTIES
C
   171 READ DRUM KDRUM,1576,ANS
       WTMOL=AAY/P
       HSUM=G(IQ2,IQ1)*T/AAY
       SSUM=0.0
       DO 183 J=1,N
       CALL BYPASS (J,1)
       IF (IPROD-2) 183,181,183
   181 SSUM=SSUM+S(J)*EN(J)
   183 CONTINUE
       SSUM=SSUM/AAY
       IMAT=IMAT-1
       CALL GAUSS (1576)
       IF (IDID-IMAT) 172,174,172
   172 CPR=CPSUM/AAY
       GAMMA=CPR/(CPR-(1.0/WTMOL))
       DLMTP=0.0
       DLMPT=0.0
       GO TO 185
   174 DLMTP=X(IQ1)
       IF (ABSF(DLMTP)-27.5) 1174,1174,172
  1174 CPR=G(IQ2,IQ2)
       DO 175 J=1,IQ1
   175 CPR=CPR-G(IQ2,J)*X(J)
       CPR=CPR/AAY
       IMAT=IMAT-1
       CALL GAUSS (1576)
       DO 179 J=1,L
   179 DLMPT=DLMPT+G(IQ1,J)*X(J)
       DLMPT=(P-DLMPT)/DLMPT
       IF (DLMPT-27.5) 180,180,172
   180 GAMMA=1.0/(1.0+DLMPT-((1.0-DLMTP)**2)/(CPR*WTMOL))
       IF (GAMMA) 172,172,185
   185 IF (IPROB-2) 186,186,207
   186 IF (IADD-2) 187,191,197
   187 WTMOLC=WTMOL
       TC=T
       PC=P
       HC=HSUM
       SO=SSUM
   188 T PI=-DLMTP/(WTMOL*CPR)
       T ETA=1000.0/(CPR*TC*1.98726)
       T SIG=-(1.0-DLMTP)/(WTMOL*CPR)
       GO TO 207
C
C      CHECK FOR CONVERGENCE AT THROAT
C
   191 DHSTAR=HC-HSUM - (GAMMA*T/(2.0*WTMOL))
       IF (ABSF(DHSTAR/(HC-HSUM))-0.4E-4) 197,197,192
   192 IF(ITROT) 193,197,193
   193 PCP(2)=PCP(2)/(1.0+2.0*DHSTAR*WTMOL/(T*(GAMMA+1.0)))
       PO=PC/PCP(IADD)
       ITROT=ITROT-1
```

```
      IF (IDEBUG) 929,194,929
  929 WRITE OUTPUT TAPE 6,923,DHSTAR,HC,HSUM,PCP(IADD)
  194 SENSE LIGHT 4
      GO TO 13
C
C     CALCULATE PERFORMANCE PARAMETERS
C
  197 SP IMP=294.98*SQRTF((HC-HSUM)*1.98726E-3)
      RHOI=RHO*SP IMP
      SUM=T/(2.0*(HC-HSUM))
      PI I=SUM*(WTMOL-WTMOLC)/(WTMOL*WTMOLC)
      ETA I=SUM*(TC-T)/(TC*T*1.98726)*1000.0
      SIG I=SUM/WTMOL
      T PI=(((WTMOLC-WTMOL)/WTMOLC)-DLMTP)/(WTMOL*CPR)
      T ETA=1000.0/(CPR*TC*1.98726)
      T SIG=-(1.0-DLMTP)/(WTMOL*CPR)
      AW=(86.4579*T)/(AAY*14.696006*SP IMP)
      AW PI=- ((1.0-DLMTP)/(WTMOLC*CPR)+1.0/GAMMA+PI I)
      AW ETA=T ETA*(1.0-DLMTP)-ETA I
      AW SIG=1.0/GAMMA-SIG I
      IF (IADD-2) 203,201,203
  201 AWT=AW
      CSTAR=32.174*PC*14.696006*AWT
      CSTRPI=1.0+AW PI
      STR ETA=AW ETA
      STR SIG=0.0
      AWT PI=AW PI
      AWT ETA=AW ETA
      AW SIG=0.0
  203 CF=32.174*SP IMP/CSTAR
      ARATIO=AW/AWT
      VACI=SP IMP+P*14.696006*AW
      RHOVAC=RHO*VACI
      VMACH=SP IMP/SQRTF(86.4579*GAMMA*T/WTMOL)
      EP PI=AW PI-AWT PI
      EP ETA=AW ETA-AWT ETA
      EP SIG=AW SIG
  207 HSUM=HSUM*1.98726
      SSUM=SSUM*1.98726
      CP=CPR*1.98726
C
C     OBTAIN COMPOSITION IN MOLE FRACTIONS
C
      SUM=P
      IF (ICOND-2) 209,213,375
  209 DO 211 J=M1,N
  211 SUM=SUM+EN(J)
  213 DO 215 J=1,N
  215 ANS(4*J+34)=EN(J)/SUM
      IF (IPROB-2) 217,217,22
  217 ANS(1)=PCP(IADD)
  218 IF (IADD-2) 220,219,219
  219 ANS(15)=CSTAR
      ANS(24)=CSTRPI
      ANS(29)=STR ETA
      ANS(34)=STR SIG
  220 ANS(2)=P
      ANS(3)=T
      K=34+4*N
C


C     PRINT OUT THE CALCULATED ANSWERS
C
      IF (IDEBUG) 1221,222,1221
 1221 WRITE OUTPUT TAPE 6,221,(ANS(I),I=1,K)
  221 FORMAT (1H ////5E20.8/5E20.8/5E20.8/4E20.8/5E20.8/5E20.8/5E20.8///
     1 (3(7X,3A6,F8.5)))
      GO TO 2223
  222 WRITE TAPE 3, (ANS(I), I=1,454)
      NO EQ=NO EQ+1
 2223 IF (IADD-2) 223,225,225
  223 IF (IPROB-2) 224,1224,1223
  224 IF (IFROZ) 1223,1224,1224
 1224 PCP(2)=((GAMMA+1.0)/2.0)**(GAMMA/(GAMMA-1.0))
      T LN=T LN+LOGF(2.0/(GAMMA+1.0))
 1223 WRITE DRUM 4,1,ANS
  225 IADD=IADD+1
      GO TO 433
C
  231 IF (NO EQ) 378,378,1231
 1231 WRITE DRUM 4,793,NO EQ
      IF (IFROZ) 232,379,235
  232 IF (IADD-2) 378,233,378
  233 IF (IDEBUG) 378,234,378
  234 CALL PONG(4)
  235 IF (IPROB-2) 237,237,239
  237 CALL PONG(3)
  239 WRITE TAPE 3,(G(I),I=1,2341)
      CALL PONG(5)
C
C     ERROR PRINT OUT
C
  305 WRITE OUTPUT TAPE 6,306,T,IADD
  306 FORMAT (17HLTHE TEMPERATURE=E12.4,34H K, IS OUT OF RANGE FOR THE P
     1OINT I5)
      IF (6000.0-T) 309,307,307
  307 IF (T-200.0) 1309,308,308
  308 GO TO 142
 1309 IF (IADD-1) 309,1310,309
 1310 IF (IPROB-2) 1311,309,309
 1311 IF (ITEST-N) 1312,1312,309
 1312 DO 1313 J=ITEST,N
      CALL BYPASS(J,1)
      IF (IPROD-2) 1315,1313,1313
 1313 CONTINUE
      GO TO 309
 1315 ITEST=J+1
      CALL BYPASS(J,3)
      GO TO 555
  309 IADD=25                                                  — see errata
      IF (SENSE LIGHT 4) 42,42
  311 WRITE OUTPUT TAPE 6,312,IMAT,IDID
  312 FORMAT (/15H1TRIED TO SOLVE I3,22H EQUATIONS, ELIMINATED I3)
      GO TO 375
  315 WRITE OUTPUT TAPE 6,316,
  316 FORMAT (/47H1RESIDUALS FROM SUBROUTINE GAUSS EXCEED  0.5E-4)
  375 IF (IDEBUG) 231,377,231
  377 IDEBUG=1
      IF (IPROB-3) 1377,555,555
 1377 PC=PC*14.696006
      GO TO 555
  378 WRITE TAPE 3,(G(I),I=1,2341)
      BACKSPACE 3
      CALL PONG(1)
```

```
  379 REWIND 4
      PAUSE 77777
      SUBROUTINE GAUSS (IWRD)
C
C     SUBROUTINE GAUSS SOLVES ANY LINEAR SET OF UP TO TWENTY EQUATIONS,
C     BY ITERATION IF NECESSARY
C
      COMMON C
      EQUIVALENCE   (G(1),        C(1)),      (G(420),      C(420))
      EQUIVALENCE   (FORM(1),     C(1)),      (FORM(15),    C(15))
      EQUIVALENCE   (ELMT(1),     C(16)),     (ELMT(15),    C(30))
      EQUIVALENCE   (DATA(1),     C(31)),     (DATA(23),    C(53))
      EQUIVALENCE   (A(1),        C(421)),    (A(1350),     C(1770))
      EQUIVALENCE   (COEFT(1),    C(421)),    (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),      C(421)),    (ANS(454),    C(874))
      EQUIVALENCE   (HSUM,        C(424)),    (SSUM,        C(425))
      EQUIVALENCE   (WTMOL,       C(426)),    (CP,          C(427))
      EQUIVALENCE   (DLMPT,       C(428)),    (DLMTP,       C(429))
      EQUIVALENCE   (GAMMA,       C(430)),    (ARATIO,      C(431))
      EQUIVALENCE   (VMACH,       C(432)),    (SP IMP,      C(433))
      EQUIVALENCE   (VACI,        C(434)),    (CF,          C(436))
      EQUIVALENCE   (RHOI,        C(437)),    (RHOVAC,      C(438))
      EQUIVALENCE   (RHO,         C(439))
      EQUIVALENCE   (T PI,        C(440)),    (PI I,        C(441))
      EQUIVALENCE   (EP PI,       C(442)),    (AW PI,       C(443))
      EQUIVALENCE   (T ETA,       C(445))
      EQUIVALENCE   (ETA I,       C(446)),    (EP ETA,      C(447))
      EQUIVALENCE   (AW ETA,      C(448)),    (T SIG,       C(450))
      EQUIVALENCE   (SIG I,       C(451)),    (EP SIG,      C(452))
      EQUIVALENCE   (AW SIG,      C(453))
      EQUIVALENCE   (EN(1),       C(1771)),   (EN(90),      C(1860))
      EQUIVALENCE   (BOX(1),      C(1771)),   (BOX(15),     C(1785))
      EQUIVALENCE   (BOF(1),      C(1786)),   (BOF(15),     C(1800))
      EQUIVALENCE   (HX,          C(1801)),   (HF,          C(1802))
      EQUIVALENCE   (VXPLS,       C(1803)),   (VXMIN,       C(1804))
      EQUIVALENCE   (VFPLS,       C(1805)),   (VFMIN,       C(1806))
      EQUIVALENCE   (EN LN(1),    C(1861)),   (EN LN(90),   C(1950))
      EQUIVALENCE   (DEL N(1),    C(1951)),   (DEL N(90),   C(2040))
      EQUIVALENCE   (COEFX(1),    C(1951)),   (COEFX(20),   C(1970))
      EQUIVALENCE   (DX(1),       C(1951)),   (DX(20),      C(1970))
      EQUIVALENCE   (HO(1),       C(2041)),   (HO(90),      C(2130))
      EQUIVALENCE   (S(1),        C(2131)),   (S(90),       C(2220))
      EQUIVALENCE   (X(1),        C(2221)),   (X(20),       C(2240))
      EQUIVALENCE   (FORMLA(1),   C(2221)),   (FORMLA(18),C(2238))
      EQUIVALENCE   (DELTA(1),    C(2241)),   (DELTA(20),   C(2260))
      EQUIVALENCE   (BO(1),       C(2261)),   (BO(15),      C(2275))
      EQUIVALENCE   (PO,          C(2276)),   (HSUBO,       C(2277))
      EQUIVALENCE   (SO,          C(2278)),   (T LN,        C(2279))
      EQUIVALENCE   (T,           C(2280)),   (AAY LN,      C(2281))
      EQUIVALENCE   (AAY,         C(2282)),   (CPSUM,       C(2283))
      EQUIVALENCE   (HC,          C(2284)),   (TC LN,       C(2285))
      EQUIVALENCE   (PCP(1),      C(2286)),   (PCP(25),     C(2310))
      EQUIVALENCE   (PROD(1),     C(2311)),   (PROD(3),     C(2313))
      EQUIVALENCE   (DATUM(1),    C(2311)),   (DATUM(3),    C(2313))
      EQUIVALENCE   (PC,          C(2314)),   (TC,          C(2315))
      EQUIVALENCE   (IPROB,       C(2316)),   (IFIXT,       C(2317))
      EQUIVALENCE   (IHS,         C(2318)),   (ICOND,       C(2319))
      EQUIVALENCE   (ISYM,        C(2320)),   (IPROD,       C(2321))
      EQUIVALENCE   (IDID,        C(2322)),   (LDRUM,       C(2323))
      EQUIVALENCE   (IDRM,        C(2323)),   (KDRUM,       C(2324))
      EQUIVALENCE   (L,           C(2325)),   (L1,          C(2326))
      EQUIVALENCE   (M,           C(2327)),   (M1,          C(2328))
      EQUIVALENCE   (N,           C(2329)),   (IQ,          C(2330))
      EQUIVALENCE   (IQ1,         C(2331)),   (IQ2,         C(2332))
      EQUIVALENCE   (IQ3,         C(2333)),   (KMAT,        C(2334))
      EQUIVALENCE   (IMAT,        C(2335)),   (IUSE,        C(2335))
      EQUIVALENCE   (IADD,        C(2336)),   (ITNUMB,      C(2337))
      EQUIVALENCE   (ITAPE,       C(2338)),   (P,           C(2339))
      EQUIVALENCE   (IDEBUG,      C(2340)),   (IFROZ,       C(2341))
C
      DIMENSION   G(20,21),    A(15,90),    EN(90),      EN LN(90)
      DIMENSION   DEL N(90),   HO(90),      S(90),       X(20)
      DIMENSION   DELTA(20),   BO(15),      PCP(25),     PROD(3)
      DIMENSION   COEFX(20),   DX(20),      FORM(15),    COEFT(15,90)
      DIMENSION   ELMT(15),    DATA(23),    DATUM(3),    FORMLA(18)
      DIMENSION   BOX(15),     BOF(15),     ANS(454),    SYSTM(15)
S I1  DEC 1
S MAX DEC 4
S IOR DEC 128
S     STZ IDID
S     CLA IUSE
S     TZE*80
S     ADD I1
S     STO IUSE1
      DO 1  K= 1, IUSE
S     STZ X(K)
S     STZ DELTA(K)
    1 CONTINUE
      ITERA= 0
      KAPUT=1
S     CLM
S     COM
S     SSP
S     STO DSUM1
C
C     SAVE MATRIX ON DRUM IDRM BEGINNING AT LOCATION IWRD
C
      WRITE DRUM IDRM, IWRD, G
C
S   2 TQO*3
S   3 TOV*4
S   4 DCT
S     NOP
C
C     BEGIN ELIMINATION OF NNTH VARIABLE
C
    6 DO 46  NN=1, IUSE
S     CLA NN
S     SUB IUSE
S     TNZ*8
S     CLA G(NN,NN)
S     TZE*23
S     TRA*31
C
C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C
    8 DO 18  I=NN, IUSE
S     CLA NN
S     STO J
S     CLA G(I,J)
```

```
S       TZE*14
S       STZ COEFX(I)
     10 J= J+1
S       CLA IUSE1
S       SUB J
S       TMI*12
S       CLA G(I,J)
S       SSP
S       LRS 35
S       ADM COEFX(I)
S       TLQ*10
S       STQ COEFX(I)
S       TRA*10
S    12 CLA COEFX(I)
S       FDP G(I,NN)
S       TQO*101
S       LLS 35
S       SSP
S       TRA*16
S   101 TOV*103
S       CLM
S       LLS 26
S       SSP
S       SUB IOR
S       TMI*14
S   103 CLM
S       TRA*15
S    14 CLM
S       COM
S    15 SSP
S    16 STO COEFX(I)
S       TOV*18
     18 CONTINUE
C
C       SEARCH FOR ROW WITH THE MINIMUM MAXIMUM COEFFICIENT
C
S    19 CLM
S       COM
S       SSP
S       STO TEMP
S       STZ I
     20 DO 22  J=NN, IUSE
S       CLA TEMP
S       LDQ COEFX(J)
S       TLQ*21
        GO TO 22
S    21 STO TEMP
        I=J
     22 CONTINUE
S       CLA I
S       TNZ*28
S    23 CLA NN
S       SUB I1
S       STO IDID
S       TRA*80
C
C       INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C       VARIABLE FROM THE REMAINING EQUATIONS
C
C       INTERCHANGE EQUATIONS I AND NN
C
S    28 CLA NN
S       SUB  I
S       TZE*31
     29 DO 30  J= NN, IUSE1
S       CLA G(I,J)
S       LDQ G(NN,J)
S       STQ G(I,J)
S       STO G(NN,J)
     30 CONTINUE
C
C       DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
C       VARIABLE FROM THE REMAINING EQUATIONS
C
     31 K= NN+1
        DO 36  J=K, IUSE1
S       CLA G(NN,J)
S       FDP G(NN,NN)
S       TQO*34
S       STQ G(NN,J)
S       TRA*35
S    34 TOV*134
S       CLM
S       LLS 26
S       SSP
S       SUB IOR
S       TMI*23
S   134 STZ G(NN,J)
S    35 TOV*36
     36 CONTINUE
S       CLA K
S       SUB IUSE1
S       TZE*46
        DO 45  I=K, IUSE
     40 DO 44  J=K, IUSE1
S       LDQ G(NN,J)
S       FMP G(I,NN)
S       TOV*42
S       CHS
S       FAD G(I,J)
S       STO G(I,J)
S       TQO*44
S       TRA*44
S    42 TQO*43
        GO TO 23
S    43 LRS 1
S       PBT
S       TRA*23
     44 CONTINUE
     45 CONTINUE
     46 CONTINUE
C
C       BACKSOLVE FOR THE VARIABLES
C
S       CLA IUSE
S       STO IDID
S       LXD IUSE, (K)
S    47 SXD K,(K)
        J= K+1
S       STZ SUM
```

```
S     CLA IUSE
S     SUB J
S     TMI*51
   48 DO 50  I= J, IUSE
      SUM= SUM + G(K,I)*DX(I)
   50 CONTINUE
   51 DX(K)= G(K,IUSE1)-SUM
      X(K)=X(K)+DX(K)
S     TIX*47 , (K), 1
      READ DRUM IDRM,IWRD, G
C
C     CALCULATE RESIDUALS (DELTA RIGHT HAND SIDE)
C
S  52 STZ DSUM
      DO 64 I=1,IUSE
S     STZ SUM
   54 DO 56 J=1,IUSE
      SUM=SUM+G(I,J)*X(J)
   56 CONTINUE
      DELTA(I)=G(I,IUSE1)-SUM
      IF (ABSF(G(I,IUSE1))-1.0) 62,62,6
   60 DELTA(I)=DELTA(I)/G(I,IUSE1)
   62 DSUM=ABSF(DELTA(I))+DSUM
   64 CONTINUE
      GO TO (66,80),KAPUT
   66 IF (DSUM-DSUM1) 74,80,68
   68 KAPUT=2
      DO 72 K=1,IUSE
   72 X(K)=X(K)-DX(K)
      GO TO 52
   74 DSUM1=DSUM
S     CLA ITERA
S     ADD I1
S     STO ITERA
S     SUB MAX
S     TZE*80
      DO 78 I=1,IUSE
      IF (ABSF(G(I,IUSE1))-1.0) 75,75,76
   75 G(I,IUSE1)=DELTA(I)
      GO TO 78
   76 G(I,IUSE1)=DELTA(I)*G(I,IUSE1)
   78 CONTINUE
      GO TO 2
   80 RETURN
```

```
      SUBROUTINE MATRIX
C
C
      COMMON C
      EQUIVALENCE   (G(1),       C(1)),     (G(420),      C(420))
      EQUIVALENCE   (FORM(1),    C(1)),     (FORM(15),    C(15))
      EQUIVALENCE   (ELMT(1),    C(16)),    (ELMT(15),    C(30))
      EQUIVALENCE   (DATA(1),    C(31)),    (DATA(23),    C(53))
      EQUIVALENCE   (A(1),       C(421)),   (A(1350),     C(1770))
      EQUIVALENCE   (COEFT(1),   C(421)),   (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),     C(421)),   (ANS(454),    C(874))
      EQUIVALENCE   (HSUM,       C(424)),   (SSUM,        C(425))
      EQUIVALENCE   (WTMOL,      C(426)),   (CP,          C(427))
      EQUIVALENCE   (DLMPT,      C(428)),   (DLMTP,       C(429))
      EQUIVALENCE   (GAMMA,      C(430)),   (ARATIO,      C(431))
      EQUIVALENCE   (VMACH,      C(432)),   (SP IMP,      C(433))
      EQUIVALENCE   (VACI,       C(434)),   (CF,          C(436))
      EQUIVALENCE   (RHOI,       C(437)),   (RHOVAC,      C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),   (PI I,        C(441))
      EQUIVALENCE   (EP PI,      C(442)),   (AW PI,       C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),   (EP ETA,      C(447))
      EQUIVALENCE   (AW ETA,     C(448)),   (T SIG,       C(450))
      EQUIVALENCE   (SIG I,      C(451)),   (EP SIG,      C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQUIVALENCE   (EN(1),      C(1771)),  (EN(90),      C(1860))
      EQUIVALENCE   (BOX(1),     C(1771)),  (BOX(15),     C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)),  (BOF(15),     C(1800))
      EQUIVALENCE   (HX,         C(1801)),  (HF,          C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)),  (VXMIN,       C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)),  (VFMIN,       C(1806))
      EQUIVALENCE   (EN LN(1),   C(1861)),  (EN LN(90),   C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)),  (DEL N(90),   C(2040))
      EQUIVALENCE   (COEFX(1),   C(1951)),  (COEFX(20),   C(1970))
      EQUIVALENCE   (DX(1),      C(1951)),  (DX(20),      C(1970))
      EQUIVALENCE   (HO(1),      C(2041)),  (HO(90),      C(2130))
      EQUIVALENCE   (S(1),       C(2131)),  (S(90),       C(2220))
      EQUIVALENCE   (X(1),       C(2221)),  (X(20),       C(2240))
      EQUIVALENCE   (FORMLA(1),  C(2221)),  (FORMLA(18),C(2238))
      EQUIVALENCE   (DELTA(1),   C(2241)),  (DELTA(20),   C(2260))
      EQUIVALENCE   (BO(1),      C(2261)),  (BO(15),      C(2275))
      EQUIVALENCE   (PO,         C(2276)),  (HSUBO,       C(2277))
      EQUIVALENCE   (SO,         C(2278)),  (T LN,        C(2279))
      EQUIVALENCE   (T,          C(2280)),  (AAY LN,      C(2281))
      EQUIVALENCE   (AAY,        C(2282)),  (CPSUM,       C(2283))
      EQUIVALENCE   (HC,         C(2284)),  (TC LN,       C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)),  (PCP(25),     C(2310))
      EQUIVALENCE   (PROD(1),    C(2311)),  (PROD(3),     C(2313))
      EQUIVALENCE   (DATUM(1),   C(2311)),  (DATUM(3),    C(2313))
      EQUIVALENCE   (PC,         C(2314)),  (TC,          C(2315))
      EQUIVALENCE   (IPROB,      C(2316)),  (IFIXT,       C(2317))
      EQUIVALENCE   (IHS,        C(2318)),  (ICOND,       C(2319))
      EQUIVALENCE   (ISYM,       C(2320)),  (IPROD,       C(2321))
      EQUIVALENCE   (IDID,       C(2322)),  (LDRUM,       C(2323))
      EQUIVALENCE   (IDRM,       C(2323)),  (KDRUM,       C(2324))
      EQUIVALENCE   (L,          C(2325)),  (L1,          C(2326))
      EQUIVALENCE   (M,          C(2327)),  (M1,          C(2328))
      EQUIVALENCE   (N,          C(2329)),  (IQ,          C(2330))
      EQUIVALENCE   (IQ1,        C(2331)),  (IQ2,         C(2332))

      EQUIVALENCE   (IQ3,        C(2333)),  (KMAT,        C(2334))
      EQUIVALENCE   (IMAT,       C(2335)),  (IUSE,        C(2335))
      EQUIVALENCE   (IADD,       C(2336)),  (ITNUMB,      C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)),  (P,           C(2339))
      EQUIVALENCE   (IDEBUG,     C(2340)),  (IFROZ,       C(2341))
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15),   COEFT(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
C
C
C     DETERMINE WHICH MATRIX IS TO BE SET UP
C     SENSE LIGHT        LIGHT ON                   LIGHT OFF
C          1          COMBUSTION TYPE            EXPANSION TYPE
C          2          ASSIGNED TEMPERATURE       UNASSIGNED TEMPERATURE
C          4          NOT CONVERGED              CONVERGED
C
      IQ1=IQ1
      IQ2=IQ2
      IQ3=IQ3
      IF (SENSE LIGHT 2) 1,4
    1 SENSE LIGHT 2
      IF (SENSE LIGHT 4) 2,3
    2 SENSE LIGHT 4
      IFIXT=1
      ISYM=IQ1
      GO TO 10
    3 IFIXT=2
      IHS=1
      ISYM=IQ2
      GO TO 10
    4 IFIXT=2
      IF (SENSE LIGHT 1) 5,6
    5 SENSE LIGHT 1
      IHS=1
      ISYM= IQ2
      GO TO 10
    6 IF (SENSE LIGHT 4) 7, 8
    7 SENSE LIGHT 4
      IHS=2
      ISYM=IQ1
      GO TO 10
    8 IHS=1
      ISYM=IQ2
C
C     CLEAR MATRIX STORAGES TO ZERO
C
   10 DO 212 I=1,IQ2
      DO 211 K=1,IQ3
      G(I,K)= 0.0
  211 CONTINUE
  212 CONTINUE
      ICOND=1
      IF (L-IQ) 14,213,14
  213 ICOND=2
C
C     BEGIN SET UP OF ITERATION MATRIX
```

```
C
   14 DO 65   J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 65,214,65
  214 IF (EN(J)) 65,65,12
C
C     CALCULATE THE ELEMENTS  R(I,K)
C
   12 DO 20  I=1, L
      IF (A(I,J)) 13,20,13
   13 TERM= A(I,J)*EN(J)
      DO 15  K=I, L
      G(I,K)= G(I,K) + A(K,J)*TERM
   15 CONTINUE
C
C     COMPLETE COLUMN  A FOR THE GAS MOLECULE
C
      G(I,IQ1)=G(I,IQ1)+TERM
   20 CONTINUE
      G(IQ1,IQ1)= G(IQ1,IQ1)+EN(J)
C
C     STATEMENT 24 IS FOR FIXED T, 30 IS FOR VARIABLE  T AND CONVERGED
C     FIXED T
C
   21 IF (IFIXT-2) 24,30,30
C
C     FOR ASSIGNED T BYPASS ENERGY ROW AND T COLUMN WHILE ITERATING
C
   24 TERM= (HO(J)-S(J))*EN(J)
      DO 25  I=1, L
      G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM
   25 CONTINUE
      G(IQ1,IQ2)=G(IQ1,IQ2)+TERM
      GO TO 65
C
C     FILL IN TEMPERATURE COLUMN AND RIGHT HAND SIDE
C
   30 TERM=HO(J)*EN(J)
      DO 35 I=1,L
      G(I,IQ2)= G(I,IQ2)+A(I,J)*TERM
   35 CONTINUE
      G(IQ1,IQ2)= G(IQ1,IQ2)+TERM
      TERM1=(HO(J)-S(J))*EN(J)
      DO 40 I=1,L
      G(I,IQ3)= G(I,IQ3)+A(I,J)*TERM1
   40 CONTINUE
      G(IQ1,IQ3)=G(IQ1,IQ3)+TERM1
C
C     STATEMENT 50 IS FOR ENTHALPY , 55 IS FOR ENTROPY EQUATION
C
   45 IF (IHS-2) 50,55,55
   50 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM
      G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*TERM1
      GO TO 65
C
C     DURING EXPANSION THE ENTROPY ROW IS FILLED IN
C
   55 TERM=S(J)*EN(J)
      DO 60  K=1,L
   60 G(IQ2,K)= G(IQ2,K)+A(K,J)*TERM

      CONTINUE
      G(IQ2,IQ1)=G(IQ2,IQ1)+TERM
      G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM
      G(IQ2,IQ3)=G(IQ2,IQ3)+(HO(J)-S(J))*TERM
   65 CONTINUE
C
C     AT THIS POINT PROCESSING OF GASEOUS PRODUCTS HAS BEEN COMPLETED
C     AND CONDENSED PHASE PROCESSING IS BEGUN
C
C     STATEMENT 70 IS FOR CONDENSED PRODUCTS, 101 IS FOR NO CONDENSED
C
   66 IF (ICOND-2) 70,101,101
   70 K=L1
      DO 100 J= M1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 100,74,100
   74 DO 75  I=1,L
      G(I,K)=A(I,J)
   75 CONTINUE
C
C     STATEMENT 80 IS FOR FIXED T, 85 IS FOR VARIABLE T AND CONVERGED
C     FIXED T
C
      IF (IFIXT-2) 80,85,85
   80 G(K,IQ2)= HO(J)-S(J)
      GO TO 95
   85 G(K,IQ2)= HO(J)
      G(K,IQ3)= HO(J)-S(J)
C
C     STATEMENT 95 IS FOR ENTHALPY, STATEMENT 90 IS FOR ENTROPY EQUATION
C
      IF (IHS-2) 95,90,90
   90 G(IQ2,K)=S(J)
   95 K= K+1
  100 CONTINUE
C
C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX BEFORE COMPLETING THE
C     CONDENSED PHASE CONTRIBUTIONS TO THE MATRIX
C
  101 DO 104 I=1,ISYM
      DO 102 J=I,ISYM
      G(J,I)=G(I,J)
  102 CONTINUE
  104 CONTINUE
C
C     THE ADDRESS OF THE NEXT INSTRUCTION IF SET DURING INITIALIZATION
C     STATEMENT 105 IS FOR CONDENSED,130  IS FOR NO CONDENSED
C
      IF (ICOND-2) 105,130,13
C
C     COMPLETE COLUMN A OF MATRIX
C
  105 DO 125 J=M1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 125,106,125
  106 DO 107 I=1,L
      G(I,IQ1)=G(I,IQ1)+A(I,J)*EN(J)
  107 CONTINUE
      IF (IFIXT-2) 125,109,109
  109 IF (IHS-2) 110,115,115
```

```
  110 G(IQ2,IQ1)= G(IQ2,IQ1)+H0(J)*EN(J)
      GO TO 125
  115 G(IQ2,IQ1)= G(IQ2,IQ1)+S(J)*EN(J)
  125 CONTINUE
  130 GO TO (131,133),IFIXT
  131 KMAT=IQ2
      GO TO 136
  133 KMAT=IQ3
  136 IMAT=KMAT-1
C
C     COMPLETE THE RIGHT HAND SIDE
C
      DO 145 I=1,IMAT
      G(I,KMAT)=G(I,KMAT)-G(I,IQ1)
  145 CONTINUE
      DO 150 I=1,L
      G(I,KMAT)= G(I,KMAT)+ AAY*B0(I)
  150 CONTINUE
      P= G(IQ1,IQ1)
  160 G(IQ1,KMAT) = G(IQ1,KMAT)+ P0
      G(IQ1,IQ1)=0.0
C
C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
C
      IF (KMAT-IQ2) 165,185,165
  165 IF (IHS-2) 166,168,168
  166 ENERGY=AAY*(HSUB0/T)
      GO TO 169
  168 ENERGY= AAY*S0+P0-P
  169 G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY
      G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM
  185 RETURN
```

```
C     MAIN PROGRAM THREE
C     FROZEN COMPOSITION EXPANSION
C
C
      COMMON C
      EQUIVALENCE    (G(1),       C(1)),      (G(420),     C(420))
      EQUIVALENCE    (FORM(1),    C(1)),      (FORM(15),   C(15))
      EQUIVALENCE    (ELMT(1),    C(16)),     (ELMT(15),   C(30))
      EQUIVALENCE    (DATA(1),    C(31)),     (DATA(23),   C(53))
      EQUIVALENCE    (A(1),       C(421)),    (A(1350),    C(1770))
      EQUIVALENCE    (COEFT(1),   C(421)),    (COEFT(1350),C(1770))
      EQUIVALENCE    (ANS(1),     C(421)),    (ANS(454),   C(874))
      EQUIVALENCE    (HSUM,       C(424)),    (SSUM,       C(425))
      EQUIVALENCE    (WTMOL,      C(426)),    (CP,         C(427))
      EQUIVALENCE    (DLMPT,      C(428)),    (DLMTP,      C(429))
      EQUIVALENCE    (GAMMA,      C(430)),    (ARATIO,     C(431))
      EQUIVALENCE    (VMACH,      C(432)),    (SP IMP,     C(433))
      EQUIVALENCE    (VACI,       C(434)),    (CF,         C(436))
      EQUIVALENCE    (RHOI,       C(437)),    (RHOVAC,     C(438))
      EQUIVALENCE    (RHO,        C(439))
      EQUIVALENCE    (T PI,       C(440)),    (PI I,       C(441))
      EQUIVALENCE    (EP PI,      C(442)),    (AW PI,      C(443))
      EQUIVALENCE    (T ETA,      C(445))
      EQUIVALENCE    (ETA I,      C(446)),    (EP ETA,     C(447))
      EQUIVALENCE    (AW ETA,     C(448)),    (T SIG,      C(450))
      EQUIVALENCE    (SIG I,      C(451)),    (EP SIG,     C(452))
      EQUIVALENCE    (AW SIG,     C(453))
      EQUIVALENCE    (EN(1),      C(1771)),   (EN(90),     C(1860))
      EQUIVALENCE    (BOX(1),     C(1771)),   (BOX(15),    C(1785))
      EQUIVALENCE    (BOF(1),     C(1786)),   (BOF(15),    C(1800))
      EQUIVALENCE    (HX,         C(1801)),   (HF,         C(1802))
      EQUIVALENCE    (VXPLS,      C(1803)),   (VXMIN,      C(1804))
      EQUIVALENCE.   (VFPLS,      C(1805)),   (VFMIN,      C(1806))
      EQUIVALENCE    (EN LN(1),   C(1861)),   (EN LN(90),  C(1950))
      EQUIVALENCE    (DEL N(1),   C(1951)),   (DEL N(90),  C(2040))
      EQ'JIVALENCE   (COEFX(1),   C(1951)),   (COEFX(20),  C(1970))
      EQUIVALENCE    (DX(1),      C(1951)),   (DX(20),     C(1970))
      EQUIVALENCE    (HO(1),      C(2041)),   (HO(90),     C(2130))
      EQUIVALENCE    (S(1),       C(2131)),   (S(90),      C(2220))
      EQUIVALENCE    (X(1),       C(2221)),   (X(20),      C(2240))
      EQUIVALENCE    (FORMLA(1),  C(2221)),   (FORMLA(18), C(2238))
      EQUIVALENCE    (DELTA(1),   C(2241)),   (DELTA(20),  C(2260))
      EQUIVALENCE    (BO(1),      C(2261)),   (BO(15),     C(2275))
      EQUIVALENCE    (PO,         C(2276)),   (HSUBO,      C(2277))
      EQUIVALENCE    (SO,         C(2278)),   (T LN,       C(2279))
      EQUIVALENCE    (T,          C(2280)),   (AAY LN,     C(2281))
      EQUIVALENCE    (AAY,        C(2282)),   (CPSUM,      C(2283))
      EQUIVALENCE    (HC,         C(2284)),   (TC LN,      C(2285))
      EQUIVALENCE    (PCP(1),     C(2286)),   (PCP(25),    C(2310))
      EQUIVALENCE    (PROD(1),    C(2311)),   (PROD(3),    C(2313))
      EQUIVALENCE    (DATUM(1),   C(2311)),   (DATUM(3),   C(2313))
      EQUIVALENCE    (PC,         C(2314)),   (TC,         C(2315))
      EQUIVALENCE    (IPROB,      C(2316)),   (IFIXT,      C(2317))
      EQUIVALENCE    (IHS,        C(2318)),   (ICOND,      C(2319))
      EQUIVALENCE    (ISYM,       C(2320)),   (IPROD,      C(2321))
      EQUIVALENCE    (IDID,       C(2322)),   (LDRUM,      C(2323))
      EQUIVALENCE    (IDRM,       C(2323)),   (KDRUM,      C(2324))
      EQUIVALENCE    (L,          C(2325)),   (L1,         C(2326))
      EQUIVALENCE    (M,          C(2327)),   (M1,         C(2328))
      EQUIVALENCE    (N,          C(2329)),   (IQ,         C(2330))

      EQUIVALENCE    (IQ1,        C(2331)),   (IQ2,        C(2332))
      EQUIVALENCE    (IQ3,        C(2333)),   (KMAT,       C(2334))
      EQUIVALENCE    (IMAT,       C(2335)),   (IUSE,       C(2335))
      EQUIVALENCE    (IADD,       C(2336)),   (ITNUMB,     C(2337))
      EQUIVALENCE    (ITAPE,      C(2338)),   (P,          C(2339))
      EQUIVALENCE    (IDEBUG,     C(2340)),   (IFROZ,      C(2341))
C
      DIMENSION    G(20,21),    A(15,90),    EN(90),      EN LN(90)
      DI'MENSION   DEL N(90),   HO(90),      S(90),       X(20)
      DIMENSION    DELTA(20),   BO(15),      PCP(25),     PROD(3)
      DIMENSION    COEFX(20),   DX(20),      FORM(15),    COEFT(15,90)
      DIMENSION    ELMT(15),    DATA(23),    DATUM(3),    FORMLA(18)
      DIMENSION    BOX(15),     BOF(15),     ANS(454),    SYSTM(15)
C
C
      NO FROZ=0
      MISSED=0
      READ DRUM 4,1,ANS
    4 IADD=1
      ITROT=3
      ALPHA=0.0
      DO 7 J=1,N
      EN(J)=ANS(4*J+34)
      IF (EN(J)) 6,6,15
   15 IF (J-M) 5,5,7
    5 EN LN(J)=LOGF(EN(J))
      ALPHA=ALPHA+EN(J)
      GO TO 7
    6 EN LN(J)=0.0
      EN(J)=0.0
    7 CONTINUE
      WTMOLF=ALPHA*WTMOL
      PC=ANS(2)
      T LN=LOGF(ANS(3))
      HC=ANS(4)/1.98726
      SO= (ANS(5)*WTMOLF/1.98726)+ALPHA*LOGF(PC/ALPHA)
      DLMPT=0.0
      DLMTP=0.0
      WRITE DRUM 4,1,ANS
C
C     BEGIN CALCULATIONS FOR CURRENT POINT
C     CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
C
   13 READ DRUM KDRUM,1,COEFT
   17 T=EXPF(T LN)
   19 IF (COEFT(7,1)-T) 21,27,27
   21 IF (COEFT(7,1)-5000.0) 23,22,451
   22 IF (IADD-2) 51,31,31
   23 BACKSPACE ITAPE
      BACKSPACE ITAPE
   25 READ TAPE ITAPE, ((COEFT(K,J),K=1,15),J=1,90)
      WRITE DRUM KDRUM,1,COEFT
      SENSE LIGHT 4
      GO TO 19
   27 IF (T-COEFT(6,1)) 29,35,35
   29 IF (300.0-COEFT(6,1)) 25,22,451
   31 IF (SENSE LIGHT 4) 38,305
C
C     LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT
C
```

```
   35 IF (IADD-2) 51,37,37
   37 IF (SENSE LIGHT 4) 38,41
   38 SENSE LIGHT 4
      DO 40 J=1,N
      IF (COEFT(8,J)) 40,39,4
   39 IF (EN(J)) 40,40,309
   40 CONTINUE
      GO TO 49
   41 DO 44 J=1,N
      IF (EN(J)) 44,44,42
   42 IF (COEFT(5,J)+20.0-T) 285,43,43
   43 IF (T-COEFT(4,J)+20.0) 295,44,44
  285 IF (5000.0-COEFT(5,J)) 44,44,311
  295 IF (COEFT(4,J)-300.0) 44,44,311
   44 CONTINUE
C
C     BEGIN ITERATION
C
   49 PCP LN=LOGF(PCP(IADD))
      READ DRUM KDRUM,1,COEFT
   51 CPSUM=0.0
      T=EXPF(T LN)
      DO 60 J=1,N
      IF (EN(J)) 60,60,57
   57 CPSUM=CPSUM+((((COEFT(12,J)*T+COEFT(11,J))*T+COEFT(10,J))*T+COEFT(
     19,J))*T+COEFT(8,J))*EN(J)
   58 HO(J)=((((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
     1+COEFT(9,J)/2.0)*T +COEFT(13,J)/T+COEFT(8,J)
   59 S(J)=((((COEFT(12,J)/4.0 )*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
     1 +COEFT(9,J))*T+COEFT(8,J)*T LN+COEFT(14,J)-EN LN(J)
   60 CONTINUE
      SUM H=0.0
      SUM S=0.0
      DO 63 J=1,N
      SUM H=SUM H+HO(J)*EN(J)
   63 SUM S=SUM S+S(J)*EN(J)
      IF (IADD-2) 81,65,65
   65 IF (SENSE LIGHT 4) 66,81
   66 SENSE LIGHT 4
   67 D LN T=(SUM S+(ALPHA*PCP LN)-SO)/CPSUM
C
C     CHECK CONVERGENCE OF THE ITERATION
C
      T LN=T LN-D LN T
      IF (ABSF(D LN T)-0.5E-4) 73,73,51
   73 IF (SENSE LIGHT 4) 17,17
   81 READ DRUM 4,1,ANS
      SUM H=T*SUM H/WTMOLF
      CPR=CPSUM/WTMOLF
      GAMMA=CPR/(CPR-(1.0/WTMOL))
      IF (IADD-2) 209,191,197
C
C     CHECK FOR CONVERGENCE AT THROAT
C
  191 DHSTAR=HC-SUM H - (GAMMA*T/(2.0*WTMOL))
      IF (ABSF(DHSTAR/(HC-SUM H))-0.4E-4) 197,197,192
  192 IF (ITROT) 193,197,193
  193 PCP(2)=PCP(2)/(1.0+2.0*DHSTAR*WTMOL/(T*(GAMMA+1.0)))
      SENSE LIGHT 4
      ITROT=ITROT-1

      GO TO 49
C
C     CALCULATE PERFORMANCE PARAMETERS
C
  197 SP IMP=294.98*SQRTF((HC-SUM H)*1.98726E-3)
      P=PC/PCP(IADD)
      AW=(86.4579*T)/(P*WTMOL*14.696006*SP IMP)
      IF (IADD-2) 203,201,203
  201 AWT=AW
      CSTAR=32.174*PC*14.696006*AWT
  203 CF=32.174*SP IMP/CSTAR
      ARATIO=AW/AWT
      VACI=SP IMP+P*14.696006*AW
      VMACH=SP IMP/SQRTF(86.4579*GAMMA*T/WTMOL)
  207 ANS(2)=P
      ANS(3)=T
  209 HSUM=SUM H*1.98726
      CP=CPR*1.98726
      ANS(1)=PCP(IADD)
      ANS(15)=CSTAR
      WRITE TAPE 3,(ANS(I),I=1,454)
      NO FROZ=NO FROZ+1
      IF (MISSED) 451,223,451
  223 IADD=IADD+1
      IF (IADD-2) 1225,224,1225
  224 PCP(2)=((GAMMA+1.0)/2.0)**(GAMMA/(GAMMA-1.0))
      T LN=T LN+LOGF(2.0/(GAMMA+1.0))
 1225 IF (IADD-25) 225,225,451
  225 IF (PCP(IADD)) 451,451,227
  227 SENSE LIGHT 4
      GO TO 49
C
C     ERROR PRINT OUT
C
  305 WRITE OUTPUT TAPE 6,306,T,IADD
  306 FORMAT (17HLTHE TEMPERATURE=E12.4,26H K, IS OUT OF RANGE,POINT I5)
      IF (6000.0-T) 449,307,307
  307 IF (T-200.0) 449,308,308
  308 GO TO 41
  449 MISSED=1
      ITROT=0
      IF (SENSE LIGHT 4) 51,51
  451 WRITE DRUM4,794,NO FROZ
      WRITE TAPE 3,(G(I),I=1,2341)
      CALL PONG(5)
  309 WRITE OUTPUT TAPE 6,310,(COEFT(I,J),I=1,3),COEFT(6,J),COEFT(7,J)
  310 FORMAT (13H6THE SPECIES 3A6,29H HAS NO DATA IN THE INTERVAL 2F9.1)
      BACKSPACE ITAPE
      BACKSPACE ITAPE
      READ TAPE ITAPE, ((COEFT(K,J),K=1,15),J=1,90)
      WRITE DRUM KDRUM,1,COEFT
      GO TO 449
  311 WRITE OUTPUT TAPE 6,312, (COEFT(I,J),I=1,3),T
  312 FORMAT (13H6THE SPECIES 3A6,19H HAS NO DATA AT T= F9.1)
      GO TO 449
```

```
C       MAIN PROGRAM FOUR
C       CHAPMAN-JOUGUET DETONATIONS
C
C
        COMMON C
        EQUIVALENCE   (G(1),       C(1)),      (G(420),      C(420))
        EQUIVALENCE   (FORM(1),    C(1)),      (FORM(15),    C(15))
        EQUIVALENCE   (ELMT(1),    C(16)),     (ELMT(15),    C(30))
        EQUIVALENCE   (DATA(1),    C(31)),     (DATA(23),    C(53))
        EQUIVALENCE   (A(1),       C(421)),    (A(1350),     C(1770))
        EQUIVALENCE   (COEFT(1),   C(421)),    (COEFT(1350),C(1770))
        EQUIVALENCE   (ANS(1),     C(421)),    (ANS(454),    C(874))
        EQUIVALENCE   (HSUM,       C(424)),    (SSUM,        C(425))
        EQUIVALENCE   (WTMOL,      C(426)),    (CP,          C(427))
        EQUIVALENCE   (DLMPT,      C(428)),    (DLMTP,       C(429))
        EQUIVALENCE   (GAMMA,      C(430)),    (ARATIO,      C(431))
        EQUIVALENCE   (VMACH,      C(432)),    (SP IMP,      C(433))
        EQUIVALENCE   (VACI,       C(434)),    (CF,          C(436))
        EQUIVALENCE   (RHOI,       C(437)),    (RHOVAC,      C(438))
        EQUIVALENCE   (RHO,        C(439))
        EQUIVALENCE   (T PI,       C(440)),    (PI I,        C(441))
        EQUIVALENCE   (EP PI,      C(442)),    (AW PI,       C(443))
        EQUIVALENCE   (T ETA,      C(445))
        EQUIVALENCE   (ETA I,      C(446)),    (EP ETA,      C(447))
        EQUIVALENCE   (AW ETA,     C(448)),    (T SIG,       C(450))
        EQUIVALENCE   (SIG I,      C(451)),    (EP SIG,      C(452))
        EQUIVALENCE   (AW SIG,     C(453))
        EQUIVALENCE   (EN(1),      C(1771)),   (EN(90),      C(1860))
        EQUIVALENCE   (BOX(1),     C(1771)),   (BOX(15),     C(1785))
        EQUIVALENCE   (BOF(1),     C(1786)),   (BOF(15),     C(1800))
        EQUIVALENCE   (HX,         C(1801)),   (HF,          C(1802))
        EQUIVALENCE   (VXPLS,      C(1803)),   (VXMIN,       C(1804))
        EQUIVALENCE   (VFPLS,      C(1805)),   (VFMIN,       C(1806))
        EQUIVALENCE   (EN LN(1),   C(1861)),   (EN LN(90),   C(1950))
        EQUIVALENCE   (DEL N(1),   C(1951)),   (DEL N(90),   C(2040))
        EQUIVALENCE   (COEFX(1),   C(1951)),   (COEFX(20),   C(1970))
        EQUIVALENCE   (DX(1),      C(1951)),   (DX(20),      C(1970))
        EQUIVALENCE   (HO(1),      C(2041)),   (HO(90),      C(2130))
        EQUIVALENCE   (S(1),       C(2131)),   (S(90),       C(2220))
        EQUIVALENCE   (X(1),       C(2221)),   (X(20),       C(2240))
        EQUIVALENCE   (FORMLA(1),  C(2221)),   (FORMLA(18),C(2238))
        EQUIVALENCE   (DELTA(1),   C(2241)),   (DELTA(20),   C(2260))
        EQUIVALENCE   (BO(1),      C(2261)),   (BO(15),      C(2275))
        EQUIVALENCE   (PO,         C(2276)),   (HSUBO,       C(2277))
        EQUIVALENCE   (SO,         C(2278)),   (T LN,        C(2279))
        EQUIVALENCE   (T,          C(2280)),   (AAY LN,      C(2281))
        EQUIVALENCE   (AAY,        C(2282)),   (CPSUM,       C(2283))
        EQUIVALENCE   (HC,         C(2284)),   (TC LN,       C(2285))
        EQUIVALENCE   (PCP(1),     C(2286)),   (PCP(25),     C(2310))
        EQUIVALENCE   (PROD(1),    C(2311)),   (PROD(3),     C(2313))
        EQUIVALENCE   (DATUM(1),   C(2311)),   (DATUM(3),    C(2313))
        EQUIVALENCE   (PC,         C(2314)),   (TC,          C(2315))
        EQUIVALENCE   (IPROB,      C(2316)),   (IFIXT,       C(2317))
        EQUIVALENCE   (IHS,        C(2318)),   (ICOND,       C(2319))
        EQUIVALENCE   (ISYM,       C(2320)),   (IPROD,       C(2321))
        EQUIVALENCE   (IDID,       C(2322)),   (LDRUM,       C(2323))
        EQUIVALENCE   (IDRM,       C(2323)),   (KDRUM,       C(2324))
        EQUIVALENCE   (L,          C(2325)),   (L1,          C(2326))
        EQUIVALENCE   (M,          C(2327)),   (M1,          C(2328))
        EQUIVALENCE   (N,          C(2329)),   (IO,          C(2330))

        EQUIVALENCE   (IQ1,        C(2331)),   (IQ2,         C(2332))
        EQUIVALENCE   (IQ3,        C(2333)),   (KMAT,        C(2334))
        EQUIVALENCE   (IMAT,       C(2335)),   (IUSE,        C(2335))
        EQUIVALENCE   (IADD,       C(2336)),   (ITNUMB,      C(2337))
        EQUIVALENCE   (ITAPE,      C(2338)),   (P,           C(2339))
        EQUIVALENCE   (IDEBUG,     C(2340)),   (IFROZ,       C(2341))
        EQUIVALENCE(P1,C(875))
        EQUIVALENCE(T1,C(876))
        EQUIVALENCE(H1,C(877))
        EQUIVALENCE(AM1,C(878))
        EQUIVALENCE(CON,C(879))
        EQUIVALENCE(GAMF,C(880))
        EQUIVALENCE(UUS,C(881))
        EQUIVALENCE(KODE,C(882))
        EQUIVALENCE(US,C(885))
        EQUIVALENCE(PPP,C(886))
        EQUIVALENCE(TTT,C(887))
        EQUIVALENCE(TE,C(888))
        EQUIVALENCE(TEM,C(889))
        EQUIVALENCE(AMD,C(890))
        EQUIVALENCE(UD,C(891))
C
        DIMENSION   G(20,21),    A(15,90),    EN(90),      EN LN(90)
        DIMENSION   DEL N(90),   HO(90),      S(90),       X(20)
        DIMENSION   DELTA(20),   BO(15),      PCP(25),     PROD(3)
        DIMENSION   COEFX(20),   DX(20),      FORM(15),    COEFT(15,90)
        DIMENSION   ELMT(15),    DATA(23),    DATUM(3),    FORMLA(18)
        DIMENSION   BOX(15),     BOF(15),     ANS(454),    SYSTM(15)
C
C
        READ DRUM 4,483,JEAN
        IF(JEAN-101)100,101,100
   100  WRITE OUTPUT TAPE 6,2
     2  FORMAT (38H1   DETONATION VELOCITY   CALCULATIONS)
        READ DRUM 4,482,KODE
        READ DRUM 4,790,OOF
        READ DRUM 4,1516,ACX,ACF,AMX,AMF
        PPP=15.0
        CON=(ACF+OOF*ACX)/(1.0+OOF)
        AM1=AMX*AMF*(1.0+OOF)/(AMX+OOF*AMF)
        WRITE OUTPUT TAPE 6,102,KODE
   102  FORMAT (4X,5HKODE=I1)
        PCP(1)=1.0/PPP
        PCP(2)=0.0
        R=1.98726
        TTT=0.0
        H1=HSUBO*R
        P1=PC
        T1=TC
        PC=PC*14.696006
        ITR=0
        JEAN=101
    20  HSUBO=H1/R+.75*T1/AM1*PPP
    22  WRITE DRUM 4,475,P1,T1,AM1,H1,ITR,R,CON,KODE,JEAN
    21  CALL PONG(2)
   101  READ DRUM 4,1,ANS
        READ DRUM  4,475,P1,T1,AM1,H1,ITR,R,CON,KODE
        GAM=GAMMA
        IF(KODE)91,92,91
    91  GAMMA=GAMMA*(1.0+DLMPT)
```

```
 92 PPP=ANS(2)/P1
    TTT=ANS(3)/T1
    E=PPP
    EE=TTT
    IF(ITR)201,200,201
200 TEMM=WTMOL/AM1
    II=0
    WRITE OUTPUT TAPE 6,203,II, PPP,TTT
    DO 202 II=1,7
    TEM=TEMM/TTT*GAMMA
    PPPP=(1.0+GAMMA)/(2.0*TEM)*
   2(1.0+SQRTF(1.0-4.0*TEM/(1.0+GAMMA)**2))
    TE=TEM/GAMMA*PPPP
    TTTT=EE-.75*R/(AM1*CP)*E+GAMMA*R/(2.*AM1*CP)*((TE**2-1.0)/TE)*PPPP
    WRITE OUTPUT TAPE 6,203,II,PPPP,TTTT
203 FORMAT(I5,2E20.8)
    IF(ABSF(PPPP-PPP)-.1)205,205,206
206 PPP=PPPP
    TTT=TTTT
202 CONTINUE
205 PCP(1)=T1*TTTT
    PC=P1*PPPP
    TC=0.0
    IPROB=3
    ITR=1
    GAMMA=GAM
    GO TO 22
201 TEMM=PPP/TTT*WTMOL/AM1
    TEM=(1.0-GAMMA*(TEMM-1.0))
    A11=1.0/PPP-GAMMA*TEMM*(1.0+DLMPT)
    A12=GAMMA*TEMM*(1.0-DLMTP)
    A21=GAMMA/2.0*(DLMPT+TEMM**2*(2.0+DLMPT))-DLMTP
    HAL=GAMMA/2.0*(TEMM**2+1.0)
    A22=HAL*(DLMTP-1.0)-WTMOL*CP/R
    B1=1.0/PPP-TEM
    B2=WTMOL/(R*ANS(3))*(HSUM-H1)-GAMMA/2.0*(TEMM**2-1.0)
    ASSIGN 51 TO JJ
 50 EEM=A11*A22-A21*A12
    X1=(B1*A22-B2*A12)/EEM
    X2=(A11*B2-A21*B1)/EEM
    GO TO JJ,(51,52,53,       59)
 51 TE=ABSF(X1)
    TEM=ABSF(X2)
    IF(TE-.4)94,94,95
 94 IF(TEM-.4)96,96,95
 96 ALAM=1.0
    GO TO 97
 95 IF(TE-TEM)93,93,98
 93 HAL=TEM
    GO TO 99
 98 HAL=TE
 99 ALAM=.4/HAL
 97 PPPP=PPP*EXPF(X1*ALAM)
    TTTT=TTT*EXPF(X2*ALAM)
301 US=91.18496 *SQRTF(GAMMA*ANS(3)/WTMOL)
    UD=TEMM*US
    PCP(1)=T1*TTTT
    PC=P1*PPPP
    TC=0.0
    IPROB=3

    TE=WTMOL/AM1
    TEM=PPPP/TTTT*TE
    E=X1**2+X2**2
    EE=SQRTF(E)
    WRITE OUTPUT TAPE 6,10,ITR
 10 FORMAT (21H0   ITERATION NUMBER=I2,10X,3HOLD,17X,3HNEW//)
    WRITE OUTPUT TAPE 6,30,PPP,PPPP,TTT,TTTT,TEMM,TEM,X1,X2,US,UD,E
   2,EE
 30 FORMAT(6X,4HP/P1,10X,1H=2E20.8/6X,4HT/T1,10X,1H=2E20.8/6X,8HRHO/RH
   1O1,6X,1H=2E20.8/6X,11HDEL LN P/P1,3X,1H=E20.8/6X,11HDEL LN T/T1,3X
   2,1H=E20.8/6X,2HUS,12X,1H=E20.8/6X,2HUD,12X,1H=E20.8/6X,1HE,13X,1H=
   3E20.8/6X,13HSQR ROOT OF E,1X,1H=E20.8)
    PPP=PPPP
    TTT=TTTT
    IF(ABSF(X1)-.5E-05)11,11,12
 11 IF(ABSF(X2)-.5E-05)13,13,12
 12 IF(ITR-10)14,13,13
 14 ITR=ITR+1
    ASSIGN 21 TO I
    GAMMA=GAM
    GO TO 22
 13 JEAN=10
    WRITE DRUM 4,483,JEAN
    P=PPP*P1
    T=TTT*T1
    US=91.18496 *SQRTF(GAMMA*T/WTMOL)
    UD=TEM*US
    WRITE OUTPUT TAPE 6,31
 31 FORMAT (17H1   FINAL ANSWERS//)
    WRITE OUTPUT TAPE 6,32,PPP,TTT,TE,TEM,P,T,WTMOL,P1,T1,AM1,US,UD
   2,CON
 32 FORMAT (6X,4HP/P1,10X,1H=E20.8/6X,4HT/T1,10X,1H=E20.8/6X,4HM/M1,10
   2X,1H=E20.8/6X,8HRHO/RHO1,6X,1H=E20.8/6X,1HP,13X,1H=E20.8/6X,1HT,13
   3X,1H=E20.8/6X,1HM,13X,1H=E20.8/6X,2HP1,12X,1H=E20.8/6X,2HT1,12X,1H
   4=E20.8/6X,2HM1,12X,1H=E20.8/6X,2HUS,12X,1H=E20.8/6X,2HUD,12X,1H=E2
   50.8/6X,2HCP,12X,1H=E20.8)
    IF(CON)41,40,41
 41 GAMF=CON/(CON-R/AM1)
    AMD=UD/(91.18496*SQRTF(GAMF*T1/AM1))
    WRITE OUTPUT TAPE 6,42,GAMF,AMD
 42 FORMAT (6X,7HGAMMA F,7X,1H=E20.8/6X,2HMD,12X,1H=E20.8)
    GO TO 150
 40 GAMF=0.0
    AMD=0.0
150 FEM=.5*(2.0+DLMPT)
    TEMM=.5*(DLMTP-1.0)
    WRITE OUTPUT TAPE 6,55
 55 FORMAT (17H0   DERIVATIVE OF,12X,4HLN P,13X,4HLN T,13X,5HLN UD/4X,
   22HBY)
    B1=1.0/PPP-GAMMA*TEM
    B2=GAMMA*  TEM**2
    ASSIGN 53 TO JJ
    GO TO 50
 53 CASE1=(FEM*X1+TEMM*X2-1.0)*UD
    X1=X1-1.0
    WRITE OUTPUT TAPE 6,81,X1,X2,CASE1
 81 FORMAT (6X,12HLNP1 AT T1,G,7X,1H=3E17.8)
    WRITE DRUM 4,1507,X1,X2,CASE1
    B1=GAMMA*TEM
    B2=-B1*TEM-WTMOL*CON/R/TTT
```

```
      ASSIGN 59 TO JJ
      GO TO 50
   59 CASE4=(FEM*X1+TEMM*X2+1.0)*UD
      X2=X2-1.0
      WRITE OUTPUT TAPE 6,84,X1,X2,CASE4
   84 FORMAT(6X,16HLNT1 AT P1,H1,M1,3X,1H=3E17.8)
      WRITE DRUM 4,1510,X1,X2,CASE4
      B1=0.0
      B2=-WTMOL/(R*T)
      ASSIGN 52 TO JJ
      GO TO 50
   52 X1=X1*1000.0
      X2=X2*1000.0
      CASE5=(FEM*X1+TEMM*X2)*UD
      WRITE OUTPUT TAPE 6,85,X1,X2,CASE5
   85 FORMAT (6X,20HH1    AT T1,P1,M1    =3E17.8)
      WRITE DRUM 4,1513,X1,X2,CASE5
      GAMMA=GAM
      IPROB=1
      UUS=91.18496*SQRTF(GAMF*T1/AM1)
      CALL OUT
      CALL PONG(1)
```

```
      SUBROUTINE OUT
C
      COMMON C
      EQUIVALENCE   (G(1),       C(1)),      (G(420),     C(420))
      EQUIVALENCE   (FORM(1),    C(1)),      (FORM(15),   C(15))
      EQUIVALENCE   (ELMT(1),    C(16)),     (ELMT(15),   C(30))
      EQUIVALENCE   (DATA(1),    C(31)),     (DATA(23),   C(53))
      EQUIVALENCE   (COEFT(1),   C(421)),    (COEFT(1350),C(1770))
      EQUIVALENCE   (ANS(1),     C(421)),    (ANS(454),   C(874))
      EQUIVALENCE   (HSUM,       C(424)),    (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,      C(426)),    (CP,         C(427))
      EQUIVALENCE   (DLMPT,      C(428)),    (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,      C(430)),    (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,      C(432)),    (SP IMP,     C(433))
      EQUIVALENCE   (VACI,       C(434)),    (CF,         C(436))
      EQUIVALENCE   (RHOI,       C(437)),    (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),    (PI I,       C(441))
      EQUIVALENCE   (EP PI,      C(442)),    (AW PI,      C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),    (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,     C(448)),    (T SIG,      C(450))
      EQUIVALENCE   (SIG I,      C(451)),    (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQUIVALENCE   (EN(1),      C(1771)),   (EN(90),     C(1860))
      EQUIVALENCE   (BOX(1),     C(1771)),   (BOX(15),    C(1785))
      EQ'JIVALENCE  (BOF(1),     C(1786)),   (BOF(15),    C(1800))
      EQUIVALENCE   (HX,         C(1801)),   (HF,         C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)),   (VXMIN,      C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)),   (VFMIN,      C(1806))
      EQUIVALENCE   (EN LN(1),   C(1861)),   (EN LN(90),  C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)),   (DEL N(90),  C(2040))
      EQUIVALENCE   (COEFX(1),   C(1951)),   (COEFX(20),  C(1970))
      EQUIVALENCE   (DX(1),      C(1951)),   (DX(20),     C(1970))
      EQUIVALENCE   (HO(1),      C(2041)),   (HO(90),     C(2130))
      EQUIVALENCE   (S(1),       C(2131)),   (S(90),      C(2220))
      EQUIVALENCE   (X(1),       C(2221)),   (X(20),      C(2240))
      EQUIVALENCE   (FORMLA(1),  C(2221)),   (FORMLA(18), C(2238))
      EQUIVALENCE   (DELTA(1),   C(2241)),   (DELTA(20),  C(2260))
      EQUIVALENCE   (BO(1),      C(2261)),   (BO(15),     C(2275))
      EQUIVALENCE   (PO,         C(2276)),   (HSUBO,      C(2277))
      EQUIVALENCE   (SO,         C(2278)),   (T LN,       C(2279))
      EQUIVALENCE   (T,          C(2280)),   (AAY LN,     C(2281))
      EQUIVALENCE   (AAY,        C(2282)),   (CPSUM,      C(2283))
      EQUIVALENCE   (HC,         C(2284)),   (TC LN,      C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)),   (PCP(25),    C(2310))
      EQUIVALENCE   (PROD(1),    C(2311)),   (PROD(3),    C(2313))
      EQUIVALENCE   (DATUM(1),   C(2311)),   (DATUM(3),   C(2313))
      EQUIVALENCE   (PC,         C(2314)),   (TC,         C(2315))
      EQUIVALENCE   (IPROB,      C(2316)),   (IFIXT,      C(2317))
      EQUIVALENCE   (IHS,        C(2318)),   (ICOND,      C(2319))
      EQUIVALENCE   (ISYM,       C(2320)),   (IPROD,      C(2321))
      EQUIVALENCE   (IDID,       C(2322)),   (LDRUM,      C(2323))
      EQUIVALENCE   (IDRM,       C(2323)),   (KDRUM,      C(2324))
      EQUIVALENCE   (L,          C(2325)),   (L1,         C(2326))
      EQUIVALENCE   (M,          C(2327)),   (M1,         C(2328))
      EQUIVALENCE   (N,          C(2329)),   (IQ,         C(2330))
      EQUIVALENCE   (IQ1,        C(2331)),   (IQ2,        C(2332))
      EQUIVALENCE   (IQ3,        C(2333)),   (KMAT,       C(2334))
      EQUIVALENCE   (IMAT,       C(2335)),   (IUSE,       C(2335))

      EQUIVALENCE   (IADD,       C(2336)),   (ITNUMB,     C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)),   (P,          C(2339))
      EQUIVALENCE   (IDEBUG,     C(2340)),   (IFROZ,      C(2341))
      EQUIVALENCE(P1,C(875))
      EQUIVALENCE(T1,C(876))
      EQUIVALENCE(H1,C(877))
      EQUIVALENCE(AM1,C(878))
      EQUIVALENCE(CON,C(879))
      EQUIVALENCE(GAMF,C(880))
      EQUIVALENCE(UUS,C(881))
      EQUIVALENCE(KODE,C(882))
      EQUIVALENCE(US,C(885))
      EQUIVALENCE(PPP,C(886))
      EQUIVALENCE(TTT,C(887))
      EQUIVALENCE(TE,C(888))
      EQUIVALENCE(TEM,C(889))
      EQUIVALENCE(AMD,C(890))
      EQUIVALENCE(UD,C(891))
      EQUIVALENCE(TITLE(1),C(892)),(TITLE(315),C(1206))
      EQUIVALENCE(AMOL(1),C(1207)),(AMOL(105),C(1311))
      EQUIVALENCE(A(1),C(1312)),(A(690),C(2001))
C
      DIMENSION   G(20,21),                EN(90),      EN LN(90)
      DIMENSION   DEL N(90),   HO(90),     S(90),       X(20)
      DIMENSION   DELTA(20),   BO(15),     PCP(25),     PROD(3)
      DIMENSION   COEFX(20),   DX(20),     FORM(15),    COEFT(15,90)
      DIMENSION   ELMT(15),    DATA(23),   DATUM(3),    FORMLA(18)
      DIMENSION   BOX(15),     BOF(15),    ANS(454),    SYSTM(15)
      DIMENSION TITLE(3,105),AMOL(1,105),A(15,46)
C
C
    2 FORMAT (9H0CASE NO.I5,F8.2,F8.2)
    3 FORMAT (1H0,64X,52HWT FRACTION  ENTHALPY   STATE  TEMP    HEAT CAP
     2ACITY/25X,16HCHEMICAL FORMULA,24X,10H(SEE NOTE),4X,7HCAL/MOL,12X,
     35HDEG K,5X,13HCAL/MOL-DEG K)
    4 FORMAT (1H0,84X,46HWT FRACTION  ENTHALPY   STATE  TEMP        CP  /
     225X,16HCHEMICAL FORMULA,44X,10H(SEE NOTE),4X,7HCAL/MOL,9X,5HDEG K)
    5 FORMAT(1H+,63X,F9.5,F12.3,4X,A1,F10.2,F11.4)
    6 FORMAT(1H+,83X,F9.5,F12.3,4X,A1,F10.2,F11.4)
    7 FORMAT (1H0,30X,4HO/F=F9.6,15H, PERCENT FUEL=F8.4,20H, EQUIVALENCE
     1 RATIO=F7.4)
   20 FORMAT      (43X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS)
   21 FORMAT (43X,45HCALCULATED USING SPECIFIC HEAT RATIO AS GAMMA)
   22 FORMAT (1H0,24HTHERMODYNAMIC PROPERITES/27X,12HUNBURNED GAS, 5X,10
     2HBURNED GAS)
   23 FORMAT (1X,6HP, ATM,20X,F12.5,3X,F12.5)
   24 FORMAT (1X,8HT, DEG K,18X,F12.2,3X,F12.1)
   25 FORMAT (1X,9HH, CAL/G ,17X,F12.1,3X,F12.1)
   26 FORMAT (1X,15HS, CAL/G-DEG K ,26X,F12.4)
   27 FORMAT (1X,11HM, MOL. WT.15X,F12.3,3X,F12.3)
   28 FORMAT (1X,16HCP, CAL/G-DEG K ,10X,F12.4,3X,F12.4)
   29 FORMAT (1X,12H(DLNM/DLNP)T,14X,F12.5,3X,F12.5)
   30 FORMAT (1X,12H(DLNM/DLNT)P,14X,F12.4,3X,F12.4)
   31 FORMAT (1X,5HGAMMA,21X,F12.4,3X,F12.4)
   32 FORMAT (1X,9HUS, M/SEC,17X,F12.1,3X,F12.1)
   33 FORMAT(1H0/1X,40HBURNED GAS COMPOSITION IN MOLE FRACTIONS//)
   34 FORMAT (1H0/1X,21HDETONATION PARAMETERS,
     22X,27H(UD IN M/SEC, H1 IN KCAL/G))
   35 FORMAT (1H0,4HP/P1,4X,1H=F7.3,5X,21H(DL(P/P1)/DLP1)T1,H1=F8.5,5X,1
     28H(DL(P/P1)/DLT1)P1=F8.5,5X,20H(DL(P/P1)/DH1)P1,T1=F8.5)
```

```
   36 FORMAT ( 1X,4HT/T1,4X,1H=F7.3,5X,21H(DL(T/T1)/DLP1)T1,H1=F8.5,5X,1
     18H(DL(T/T1)/DLT1)P1=F8.5,5X,20H(DL(T/T1)/DH1)P1,T1=F8.5)
   37 FORMAT (1X,4HM/M1,4X,1H=F7.4)
   38 FORMAT (1X,9HRHO/RHO1=F7.4)
   39 FORMAT (1X,9HMACH NO.=F7.4)
   40 FORMAT (1X,9HUD      =F7.1,5X,16H(D UD/DLP1)T1,H1,4X,1H=F8.2,5X,13
     1H(D UD/DLT1)P14X,1H=F8.2,5X,15H(D UD/DH1)P1,T1,4X,1H=F8.2)
      READ DRUM 4,789,KASE,OOF,PERCF,EQUIV
      READ DRUM 4,1503,KD
      READ DRUM 4,1700,N
 1000 WRITE OUTPUT TAPE 6,18
   18 FO?MAT (1H1)
  552 REWIND 3
  300 READ TAPE 3,(ANS(I),I=1,454)
      HAL=P1*14.696006
      I=1
      J=38
      DO 350 JJ=1,N
      AMOL(1,I)=ANS(J)
      J=J+4
  350 I=I+1
      WRITE OUTPUT TAPE 6,20
      IF(KODE)351,352,351
  351 WRITE OUTPUT TAPE 6,21
  352 CONTINUE
S     STZ ZERO
  106 J=34
      DO 104 I=1,N
      DO 105 II=1,3
      KK=J+II
  105 TITLE(II,I)=ANS(KK)
  104 J=J+4
      READ DRUM 4,795,A,NF,NO,NE,ELMT
      ASSIGN 90 TO JEAN
   92 WRITE OUTPUT TAPE 6,2,KASE,HAL,T1
      GO TO JEAN,(90,91)
   90 IF(KD)93,94,93
   94 WRITE OUTPUT TAPE 6,3
      GO TO 97
   93 WRITE OUTPUT TAPE 6,4
   97 IF(NF)451,450,451
  451 DO 100 I=1,NF
      II=I
      MM=15
      CALL SPEC(II,MM,A,ELMT,KD)
      IF(KD)401,400,401
  400 WRITE OUTPUT TAPE 6,5,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
      GO TO 100
  401 WRITE OUTPUT TAPE 6,6,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
  100 CONTINUE
  450 IF(NO)453,452,453
  453 DO 101 I=1,NO
      II=I
      MM=0
      CALL SPEC(II,MM,A,ELMT,KD)
      IF(KD)411,410,411
  410 WRITE OUTPUT TAPE 6,5,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
      GO TO 101
  411 WRITE OUTPUT TAPE 6,6,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
  101 CONTINUE

  452 CONTINUE
      WRITE OUTPUT TAPE 6,7,OOF,PERCF,EQUIV
      WRITE OUTPUT TAPE 6,22
      WRITE OUTPUT TAPE 6,23,P1,P
      WRITE OUTPUT TAPE 6,24,T1,T
      WRITE OUTPUT TAPE 6,25,H1,ANS(4)
      WRITE OUTPUT TAPE 6,26,ANS(5)
      WRITE OUTPUT TAPE 6,27,AM1,ANS(6)
      WRITE OUTPUT TAPE 6,28,CON,ANS(7)
      WRITE OUTPUT TAPE 6,29,ZERO,ANS(8)
      WRITE OUTPUT TAPE 6,30,ZERO,ANS(9)
      WRITE OUTPUT TAPE 6,31,GAMF,ANS(10)
      WRITE OUTPUT TAPE6,32,UUS,US
      WRITE OUTPUT TAPE 6,33
      CALL COMP(AMOL,TITLE,1,N,2)
      WRITE OUTPUT TAPE 6,34
      READ DRUM 4,1507,A1,A2,A3,A4,A5,A6,A7,A8,A9
      WRITE OUTPUT TAPE 6,35,PPP,A1,A4,A7
      WRITE OUTPUT TAPE 6,36,TTT,A2,A5,A8
      WRITE OUTPUT TAPE 6,40,UD,A3,A6,A9
      WRITE OUTPUT TAPE 6,37,TE
      WRITE OUTPUT TAPE 6,38,TEM
      WRITE OUTPUT TAPE 6,39,AMO
  207 WRITE OUTPUT TAPE 6,16
   16 FORMAT (1H0,30X,16HINPUT, G-ATOMS/G//)
      READ DRUM 4,1702,BOX,BOF,BO
      READ DRUM 4,1487,NE,ELMT
      IF(NE-8)80,80,81
   80 KK=1
      KKK=NE
      LOOP=1
      GO TO 82
   81 KK=1
      KKK=8
      LOOP=2
   82 DO 85 J=1,LOOP
      WRITE OUTPUT TAPE 6,11,(ELMT(I),I=KK,KKK)
   11 FORMAT (11X,8(6X,A2,7X))
      WRITE OUTPUT TAPE 6,12,(BOF (I),I=KK,KKK)
   12 FORMAT (5H FUEL,6X,8E15.7)
      WRITE OUTPUT TAPE 6,13,(BOX (I),I=KK,KKK)
   13 FORMAT (8H OXIDANT,3X,8E15.7)
      WRITE OUTPUT TAPE 6,14,(BO  (I),I=KK,KKK)
   14 FORMAT (11H PROPELLANT,8E15.7)
      IF (LOOP-1) 86,85,86
   86 KK=9
      KKK=NE
      WRITE OUTPUT TAPE 6,15
   15 FORMAT(1H0)
   85 CONTINUE
      ASSIGN 91 TO JEAN
      GO TO 92
   91 WRITE OUTPUT TAPE 6,119
  119 FORMAT (6HONOTE.,2X,71HWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND
     1OF OXIDANT IN TOTAL OXIDANTS)
      RETURN
```

```
      SUBROUTINE ONCE(N,M,TITLE)
C     OUTPUTS ODD PRODUCTS
C
C
      DIMENSION M(105),TITLE(3,105) ,TEM(10),FMT(3)
SA    ALF      1X,2
SB    ALF     14X,2
SC    ALF     27X,2
SD    ALF     40X,2
SE    ALF     53X,2
SAA   ALF     66X,2
SBB   ALF     79X,2
SCC   ALF     92X,2
SDD   ALF    105X,2
SEE   ALF    118X,2
SFOR  ALF    (1H+,
SAPE  ALF    A6)
      WRITE OUTPUT TAPE 6,1
      FMT(1)=FOR
      FMT(3)=APE
      TEM(1)=A
      TEM(2)=B
      TEM(3)=C
      TEM(4)=D
      TEM(5)=E
      TEM(6)=AA
      TEM(7)=BB
      TEM(8)=CC
      TEM(9)=DD
      TEM(10)=EE
      K=0
      KK=10
      DO 10 I=1,N
      J=M(I)
      IF(I-KK) 20,20,21
   20 K=K+1
      GO TO 5
   21 K=1
      KK=KK+10
      WRITE OUTPUT TAPE 6,1
    1 FORMAT (1H )
    5 FMT(2)=TEM(K)
      WRITE OUTPUT TAPE 6,FMT,TITLE(2,J),TITLE(3,J)
   10 CONTINUE
      RETURN

      SUBROUTINE SPEC(I,M,A,ELMT,KONT)
C     OUTPUTS FUEL AND OXIDANT FROM SUBROUTINE INPUT
C
C
      DIMENSION A(15,46),TEM(5),ANAME(5),ELMT(15)
      DIMENSION II(5)
   55 FORMAT (10X,4HFUEL)
   66 FORMAT (10X,7HOXIDANT)
      IF (M ) 2,1,2
    1 WRITE OUTPUT TAPE 6,66
      GO TO 3
    2 WRITE OUTPUT TAPE 6,55
    3 K=0
      DO 11 J=1,15
      KK=I+M
      IF(A(J,KK))12,11,12
   12 K=K+1
      TEM(K)=A(J,KK)
      ANAME(K)=ELMT(J)
      II(K)=TEM(K)
   11 CONTINUE
      IF(KONT)21,20,21
   20 WRITE OUTPUT TAPE 6,4,(ANAME(I),II(I),I=1,K)
    4 FORMAT(1H+,18X,5(A2,I2,5X))
      GO TO 13
   21 WRITE OUTPUT TAPE 6,5,(ANAME(I),TEM(I),I=1,K)
    5 FORMAT (1H+,18X,5(A2,F8.5,3X))
   13 RETURN
```

```
      SUBROUTINE COMP(AMOL,TITLE,IN,N,ME)
C     OUTPUTS COMPOSITION
C
C
      DIMENSION AMOL(1 ,105),TITLE(3,105),IOMIT(105),ILESS(105)
      DIMENSION FMT(4),TEM(4)
SA    ALF   (1H+,
SB    ALF   A6,F8.
SC    ALF   5)
SD    ALF     7X,2
SE    ALF    36X,2
SF    ALF    64X,2
SG    ALF    92X,2
SOMIT ALF   OMIT
    1 FORMAT (1X,2A6,2X,13F9.5)
    3 FORMAT (1H0,    118HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT W
     1HOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDI
     2TIONS//)
    4 FORMAT (1H0,     59HPRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM
     1CALCULATIONS//)
      TEM(1)=D
      TEM(2)=E
      TEM(3)=F
      TEM(4)=G
      FMT(1)=A
      FMT(3)=B
      FMT(4)=C
      K=0
      KK=4
      IOM=0
      ILE=0
      IF(ME-1)61,60,61
   61 WRITE OUTPUT TAPE 6,44
   60 II=0
      DO 9 I=1,N
S     CLA TITLE (1,I)
S     SUB OMIT
S     TNZ *10
      IOM=IOM+1
      IOMIT(IOM)=I
      GO TO 9
   10 DO 11 J=1,IN
      IF(AMOL(J,I)-.5E-05)11,12,12
   11 CONTINUE
      ILE=ILE+1
      ILESS(ILE)=I
      GO TO 9
   12 IF(ME-1)51,50,51
   50 WRITE OUTPUT TAPE 6,1 ,TITLE(2,I),TITLE(3,I),(AMOL(JJ,I),JJ=1,IN)
      GO TO 9
   51 II=II+1
      IF(II-KK)200,200,201
  200 K=K+1
      GO TO 5
  201 K=1
      KK=KK+4
      WRITE OUTPUT TAPE 6,44
   44 FORMAT (1H )
    5 FMT(2)=TEM(K)
      WRITE OUTPUT TAPE 6,FMT,TITLE(2,I),TITLE(3,I),AMOL(1,I)

    9 CONTINUE
      IF(ILE) 21,20,21
   21 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,3
      CALL ONCE(ILE,ILESS,TITLE)
   20 IF(IOM) 31,30,31
   31 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,4
      CALL ONCE (IOM,IOMIT,TITLE)
   30 RETURN
```

```
C       MAIN PROGRAM FIVE
C
C       OUTPUT PROGRAM
C
C
        COMMON C
        EQUIVALENCE(ANS(1),      C(25)),     (ANS(454),   C(478))
        EQUIVALENCE(TITLE(1),    C(479)),    (TITLE(315), C(793))
        EQUIVALENCE(PAR(1),      C(794)),    (PAR(208),   C(1001))
        EQUIVALENCE(DER(1),      C(1002)),   (DER(169),   C(1170))
        EQUIVALENCE(AMOL(1),     C(1171)),   (AMOL(1365), C(2535))
        EQUIVALENCE(A(1),        C(794)),    (A(690),     C(1483))
        EQUIVALENCE(ELMT(1),     C(1484)),   (ELMT(15),   C(1498))
        EQUIVALENCE(BOX(1),      C(1499)),   (BOX(15),    C(1513))
        EQUIVALENCE(BOF(1),      C(1514)),   (BOF(15),    C(1528))
        EQUIVALENCE(BO(1),       C(1529)),   (BO(15),     C(1543))
        EQUIVALENCE(II,          C(2536)),   (MM,         C(2537))
        EQUIVALENCE(KD,          C(2538)),   (IN,         C(2539))
        EQUIVALENCE(N ,          C(2540)),   (LEN,        C(2541))
        EQUIVALENCE(ME,          C(2542)),   (MAY,        C(2543))
        EQUIVALENCE(NANA,        C(2544)),   (IPROB,      C(2545))
        EQUIVALENCE(NF,          C(1)),      (NO,         C(2))
        EQUIVALENCE(NE,          C(3)),      (KK,         C(19))
        EQUIVALENCE(KKK,         C(20)),     (LOOP,       C(21))
        EQUIVALENCE(KTAPE,       C(2546))
        DIMENSION         TITLE(3,105),PAR(13,16),DER(13,13),AMOL(13,105),
       2              A(15,46),ELMT(15)
       3,ANS(454)
        DIMENSION BOX(15),BOF(15),BO(15)
        DIMENSION ASOL(13)
C
C       MAIN CONTROL FOR ONE OR TWO LOOPS
C
SEXIT ALF   EXIT
      2 FORMAT (9HOCASE NO.I5,F8.1,F7.3)
      3 FORMAT (1H0,64X,46HWT FRACTION  ENTHALPY   STATE  TEMP    DENSITY/
       225X,16HCHEMICAL FORMULA,24X,10H(SEE NOTE),4X,7HCAL/MOL,10X,
       35HDEG K,4X,4HG/CC)
      4 FORMAT (1H0,84X,46HWT FRACTION  ENTHALPY   STATE  TEMP    DENSITY/
       2          25X,16HCHEMICAL FORMULA,44X,10H(SEE NOTE),4X,7HCAL/MOL,
       3          8X,5HDEG K,4X,4HG/CC)
      5 FORMAT(1H+,63X,F9.5,F12.3,4X,A1,F10.2,F11.6)
      6 FORMAT(1H+,83X,F9.5,F12.3,4X,A1,F10.2,F11.6)
      7 FORMAT (1H0,30X,4HO/F=F9.6,15H, PERCENT FUEL=F8.4,20H, EQUIVALENCE
       1 RATIO=F7.4,10H, DENSITY=F7.4)
        READ DRUM 4,789,KASE,OOF,PERCF,EQUIV,NOEQ,NOFROZ
        READ DRUM 4,1503,KD
        READ DRUM 4,1700,N,IPROB
        DO 60 I=1,13
S       CLA EXIT
S    60 STO ASOL(I)
        IF(IPROB-2)550,550,551
    550 NANA=2
        GO TO 552
    551 NANA=1
    552 REWIND 3
        KANE=NANA
        DO 200 ME=1,KANE
        KTAPE=0
    300 READ TAPE 3,(ANS(I),I=1,454)

        KTAPE=KTAPE+1
        HAL=ANS(2)*14.696006
        HALL=ANS(19)
        IF(ME-1)202,201,202
    201 LEN=NOEQ
        GO TO 203
    202 LEN=NOFROZ
    203 IF(LEN-13)102,102,103
    102 KODE=0
        GO TO 106
    103 KONT=0
        KODE=13
    106 J=34
        DO 104 I=1,N
        DO 105 II=1,3
        KK=J+II
    105 TITLE(II,I)=ANS(KK)
    104 J= J+4
        MAY=1
   1000 WRITE OUTPUT TAPE 6,18
     18 FORMAT (1H1)
        CALL HEAD
        READ DRUM 4,795,A,NF,NO,NE,ELMT
        ASSIGN 90 TO JEAN
     92 WRITE OUTPUT TAPE 6,2,KASE,HAL,OOF
        GO TO JEAN,(90,91)
     90 IF(KD)93,94,93
     94 WRITE OUTPUT TAPE 6,3
        GO TO 97
     93 WRITE OUTPUT TAPE 6,4
     97 IF(NF)351,350,351
    351 DO 100 I=1,NF
        II=I
        MM=15
        CALL SPEC
        IF(KD)401,400,401
    400 WRITE OUTPUT TAPE 6,5,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
        GO TO 100
    401 WRITE OUTPUT TAPE 6,6,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
    100 CONTINUE
    350 IF(NO)353,352,353
    353 DO 101 I=1,NO
        II=I
        MM=0
        CALL SPEC
        IF(KD)411,410,411
    410 WRITE OUTPUT TAPE 6,5,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
        GO TO 101
    411 WRITE OUTPUT TAPE 6,6,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
    101 CONTINUE
    352 CONTINUE
        WRITE OUTPUT TAPE 6,7,OOF,PERCF,EQUIV,HALL
        IF(KODE) 51,50,51
     50 IN=LEN
        GO TO 56
     51 IF(KONT) 53,52,53
     52 IN=KODE
        KONT=1
        GO TO 56
     53 IN=LEN -13
```

```
      KODE=0
   56 CALL READ
      IF(IPROB-2)600,600,601
  601 WRITE OUTPUT TAPE 6,602
  602 FORMAT (37H0EQUILIBRIUM THERMODYNAMIC PROPERTIES)
      CALL PERPAR
      GO TO 206
  600 WRITE OUTPUT TAPE 6,8
    8 FORMAT (11H0PARAMETERS)
      IF(MAY-1)64,63,64
   63 KK=IN-2
      WRITE OUTPUT TAPE 6,61,(ASOL(I),I=1, KK)
   61 FORMAT (1H0,16X,7HCHAMBER,4X,7HTHROAT ,10(3X,A6),3X,A4)
      GO TO 65
   64 WRITE OUTPUT TAPE 6,66,(ASOL(I),I=1,IN)
   66 FORMAT (1H0,15X,13(3X,A6))
   65 CONTINUE
      CALL PERPAR
      IF(ME-1)206,205,206
  205 WRITE OUTPUT TAPE 6,99
   99 FORMAT(1H )
      WRITE OUTPUT TAPE 6,9
    9 FORMAT (12H0DERIVATIVES)
      IF(MAY-1) 503,502,503
  503 CALL PERDER
      GO TO 504
  502 CALL PERDEY
  504 CONTINUE
  206 WRITE OUTPUT TAPE 6,99
      WRITE OUTPUT TAPE 6,10
   10 FORMAT (15H0MOLE FRACTIONS//)
      CALL COMP
  207 WRITE OUTPUT TAPE 6,16
   16 FORMAT (1H0,30X,16HINPUT, G-ATOMS/G//)
      READ DRUM 4,1702,B0X,B0F,B0
      READ DRUM 4,1487,NE,ELMT
      IF(NE-8)80,80,81
   80 KK=1
      KKK=NE
      LOOP=1
      GO TO 82
   81 KK=1
      KKK=8
      LOOP=2
   82 DO 85 J=1,LOOP
      WRITE OUTPUT TAPE 6,11,(ELMT(I),I=KK,KKK)
   11 FORMAT (11X,8(6X,A2,7X))
      WRITE OUTPUT TAPE 6,12,(B0F (I),I=KK,KKK)
   12 FORMAT (5H FUEL,6X,8E15.7)
      WRITE OUTPUT TAPE 6,13,(B0X (I),I=KK,KKK)
   13 FORMAT (8H OXIDANT,3X,8E15.7)
      WRITE OUTPUT TAPE 6,14,(B0  (I),I=KK,KKK)
   14 FORMAT (11H PROPELLANT,8E15.7)
      IF (LOOP-1) 86,85,86
   86 KK=9
      KKK=NE
      WRITE OUTPUT TAPE 6,15
   15 FORMAT(1H0)
   85 CONTINUE
      ASSIGN 91 TO JEAN

      GO TO 92
   91 WRITE OUTPUT TAPE 6,119
  119 FORMAT (6H0NOTE.,2X,71HWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND
     1OF OXIDANT IN TOTAL OXIDANTS)
      IF(KODE)96,95,96
   96 MAY=MAY+1
      GO TO 1000
   95 IF(NANA-1)208,200,208
  208 NANA=0
  200 CONTINUE
      CALL PONG(1)
C
C
C
      SUBROUTINE SPEC
C     OUTPUTS FUEL AND OXIDANT FROM SUBROUTINE INPUT
C
C
      COMMON C
      EQUIVALENCE(TEM(1),      C(18)),     (TEM(5),      C(22))
      EQUIVALENCE(ANAME(1),    C(6)),      (ANAME(5),    C(10))
      EQUIVALENCE(II(1),       C(11)),     (II(5),       C(15))
      EQUIVALENCE(K,           C(16)),     (KK,          C(17))
      EQUIVALENCE(A(1),        C(794)),    (A(690),      C(1483))
      EQUIVALENCE(ELMT(1),     C(1484)),   (ELMT(15),    C(1498))
      EQUIVALENCE(I,           C(2536)),   (M,           C(2537))
      EQUIVALENCE(KONT,        C(2538))
      DIMENSION A(15,46),TEM(5),ANAME(5),ELMT(15)
      DIMENSION II(5)
   55 FORMAT (10X,4HFUEL)
   66 FORMAT (10X,7HOXIDANT)
      IF (M ) 2,1,2
    1 WRITE OUTPUT TAPE 6,66
      GO TO 3
    2 WRITE OUTPUT TAPE 6,55
    3 K=0
      DO 11 J=1,15
      KK=I+M
      IF(A(J,KK))12,11,12
   12 K=K+1
      TEM(K)=A(J,KK)
      ANAME(K)=ELMT(J)
      II(K)=TEM(K)
   11 CONTINUE
      IF(KONT)21,20,21
   20 WRITE OUTPUT TAPE 6,4,(ANAME(I),II(I),I=1,K)
    4 FORMAT(1H+,18X,5(A2,I2,5X))
      GO TO 13
   21 WRITE OUTPUT TAPE 6,5,(ANAME(I),TEM(I),I=1,K)
    5 FORMAT (1H+,18X,5(A2,F8.5,3X))
   13 RETURN
C
C
C
      SUBROUTINE HEAD
C     OUTPUTS PROPER HEADING ACCORDING TO PROBLEM NUMBER
C
C
      COMMON C
      EQUIVALENCE(IPROB,       C(2545)),   (ME,          C(2542))
```

```
100 FORMAT (     25X,80HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB
   2RIUM COMPOSITION DURING EXPANSION)
200 FORMAT (     25X,75HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
   2COMPOSITION DURING EXPANSION)
300 FORMAT (     25X,80HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB
   2RIUM COMPOSITION DURING EXPANSION/44X,28HFROM AN ASSIGNED TEMPERAT
   3URE)
400 FORMAT (     25X,75HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
   2COMPOSITION DURING EXPANSION/44X,28HFROM AN ASSIGNED TEMPERATURE)
500 FORMAT (     25X,74HTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE
   2D PRESSURE AND TEMPERATURES)
600 FORMAT (     25X,74HTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE
   2D TEMPERATURE AND PRESSURES)
    IF(IPROB-2)1,2,10
 10 IF(IPROB-4)3,4,4
  1 IF(ME-1)12,11,12
 11 WRITE OUTPUT TAPE 6,100
    RETURN
 12 WRITE OUTPUT TAPE 6,200
    RETURN
  2 IF(ME-1)14,13,14
 13 WRITE OUTPUT TAPE 6,300
    RETURN
 14 WRITE OUTPUT TAPE 6,400
    RETURN
  3 WRITE OUTPUT TAPE 6,500
    RETURN
  4 WRITE OUTPUT TAPE 6,600
    RETURN
C
C
C
      SUBROUTINE PERDER
C     OUTPUTS PERFORMANCE DERIVATIVES
C
C
      COMMON C
      EQUIVALENCE(PER(1),     C(1002)),  (PER(169),   C(1170))
      EQUIVALENCE(IN,         C(2539))
      DIMENSION PER(13,13)
    1 FORMAT (15H0(DLI/DLPC)PC/P13F9.5)
    2 FORMAT (15H (DLT/DLPC)PC/P13F9.5)
    3 FORMAT (16H (DLAR/DLPC)PC/PF8.5,12F9.5)
    4 FORMAT (16H (DLCS/DLPC)PC/PF8.5,12F9.5)
    5 FORMAT (15H0(DLI/DHC)PC/P*13F9.5)
    6 FORMAT (15H (DLT/DHC)PC/P*13F9.5)
    7 FORMAT (16H (DLAR/DHC)PC/P*F8.5,12F9.5)
    8 FORMAT (16H (DLCS/DHC)PC/P*F8.5,12F9.5)
    9 FORMAT (16H *(HC IN KCAL/G))
   10 FORMAT (13H0(DLI/DLPCP)S,2X,13F9.5)
   11 FORMAT (13H (DLT/DLPCP)S,2X,13F9.5)
   12 FORMAT (15H (DLAR/DLPCP)S 13F9.5)
      WRITE OUTPUT TAPE 6,1,(PER(I,2),I=1,IN)
      WRITE OUTPUT TAPE 6,2,(PER(I,1),I=1,IN)
      WRITE OUTPUT TAPE 6,3,(PER(I,3),I=1,IN)
      WRITE OUTPUT TAPE 6,4,(PER(I,5),I=1,IN)
      WRITE OUTPUT TAPE 6,5,(PER(I,7),I=1,IN)
      WRITE OUTPUT TAPE 6,6,(PER(I,6),I=1,IN)
      WRITE OUTPUT TAPE 6,7,(PER(I,8),I=1,IN)
      WRITE OUTPUT TAPE 6,8,(PER(I,10),I=1,IN)

      WRITE OUTPUT TAPE 6,9
      WRITE OUTPUT TAPE 6,10,(PER(I,12),I=1,IN)
      WRITE OUTPUT TAPE 6,11,(PER(I,11),I=1,IN)
      WRITE OUTPUT TAPE 6,12,(PER(I,13),I=1,IN)
      RETURN
C
C
C
      SUBROUTINE PERDEY
C     OUTPUTS PERFORMANCE DERIVATIVES
C
C
      COMMON C
      EQUIVALENCE(PER(1),     C(1002)),  (PER(169),   C(1170))
      EQUIVALENCE(IN,         C(2539))
      DIMENSION PER(13,13)
    1 FORMAT (15H0(DLI/DLPC)PC/P,9X,12F9.5)
    2 FORMAT (15H (DLT/DLPC)PC/P13F9.5)
    3 FORMAT (16H (DLAR/DLPC)PC/P,8X,12F9.5)
    4 FORMAT (16H (DLCS/DLPC)PC/P,8X,12F9.5)
    5 FORMAT (15H0(DLI/DHC)PC/P*,9X,12F9.5)
    6 FORMAT (15H (DLT/DHC)PC/P*13F9.5)
    7 FORMAT (16H (DLAR/DHC)PC/P*,8X,12F9.5)
    8 FORMAT (16H (DLCS/DHC)PC/P*,8X,12F9.5)
    9 FORMAT (16H *(HC IN KCAL/G))
   10 FORMAT (13H0(DLI/DLPCP)S,11X,12F9.5)
   11 FORMAT (13H (DLT/DLPCP)S,2X,13F9.5)
   12 FORMAT (15H (DLAR/DLPCP)S,9X,12F9.5)
      WRITE OUTPUT TAPE 6,1,(PER(I,2),I=2,IN)
      WRITE OUTPUT TAPE 6,2,(PER(I,1),I=1,IN)
      WRITE OUTPUT TAPE 6,3,(PER(I,3),I=2,IN)
      WRITE OUTPUT TAPE 6,4,(PER(I,5),I=2,IN)
      WRITE OUTPUT TAPE 6,5,(PER(I,7),I=2,IN)
      WRITE OUTPUT TAPE 6,6,(PER(I,6),I=1,IN)
      WRITE OUTPUT TAPE 6,7,(PER(I,8),I=2,IN)
      WRITE OUTPUT TAPE 6,8,(PER(I,10),I=2,IN)
      WRITE OUTPUT TAPE 6,9
      WRITE OUTPUT TAPE 6,10,(PER(I,12),I=2,IN)
      WRITE OUTPUT TAPE 6,11,(PER(I,11),I=1,IN)
      WRITE OUTPUT TAPE 6,12,(PER(I,13),I=2,IN)
      RETURN
C
C
C
      SUBROUTINE READ
C     SORTS WHAT IS ON TAPE 3
C
C
      COMMON C
      EQUIVALENCE(N,          C(1)),     (J,          C(2))
      EQUIVALENCE(ANS(1),     C(25)),    (ANS(454),   C(478))
      EQUIVALENCE(PAR(1),     C(794)),   (PAR(208),   C(1001))
      EQUIVALENCE(DER(1),     C(1002)),  (DER(169),   C(1170))
      EQUIVALENCE(AMOL(1),    C(1171)),  (AMOL(1365), C(2535))
      EQUIVALENCE(IN,         C(2539)),  (LEN,        C(2541))
      EQUIVALENCE(KTAPE,      C(2546))
      EQUIVALENCE(NN,          C(2540))
      DIMENSION PAR(13,16),DER(13,13),AMOL(13,105),ANS(454)
      DO 1 I=1,IN
      DO 2 J=1,16
```

```
      2 PAR(I,J)=ANS(J)
        N=1
        DO 3 J=20,32
        DER(I,N)=ANS(J)
      3 N=N+1
        N=1
        J=38
        DO 4 JJ=1,NN
        AMOL(I,N)=ANS(J)
        J=J+4
      4 N=N+1
        IF(KTAPE-LEN)100,1,100
    100 READ TAPE 3,(ANS(K),K=1,454)
        KTAPE=KTAPE+1
      1 CONTINUE
        RETURN
C
C
C
        SUBROUTINE ONCE (N,M)
C       OUTPUTS ODD PRODUCTS
C
C
        COMMON C
        EQUIVALENCE(TEM(1),      C(1)),      (TEM(10),     C(10))
        EQUIVALENCE(FMT(1),      C(11)),     (FMT(3),      C(13))
        EQUIVALENCE(K,           C(14)),     (KK,          C(15))
        EQUIVALENCE(TITLE(1),    C(479)),    (TITLE(315),  C(793))
        DIMENSION M(105),TITLE(3,105) ,TEM(10),FMT(3)
SA      ALF      1X,2
SB      ALF     14X,2
SC      ALF     27X,2
SD      ALF     40X,2
SE      ALF     53X,2
SAA     ALF     66X,2
SBB     ALF     79X,2
SCC     ALF     92X,2
SDD     ALF    105X,2
SEE     ALF    118X,2
SFOR    ALF    (1H+,
SAPE    ALF    A6)
        WRITE OUTPUT TAPE 6,1
        FMT(1)=FOR
        FMT(3)=APE
        TEM(1)=A
        TEM(2)=B
        TEM(3)=C
        TEM(4)=D
        TEM(5)=E
        TEM(6)=AA
        TEM(7)=BB
        TEM(8)=CC
        TEM(9)=DD
        TEM(10)=EE
        K=0
        KK=10
        DO 10 I=1,N
        J=M(I)
        IF(I-KK) 20,20,21
     20 K=K+1

        GO TO 5
     21 K=1
        KK=KK+10
        WRITE OUTPUT TAPE 6,1
      1 FORMAT (1H )
      5 FMT(2)=TEM(K)
        WRITE OUTPUT TAPE 6,FMT,TITLE(2,J),TITLE(3,J)
     10 CONTINUE
        RETURN
C
C
C
        SUBROUTINE COMP
C       OUTPUTS COMPOSITION
C
C
        COMMON C
        EQUIVALENCE(FMT(1),      C(1)),      (FMT(4),      C(4))
        EQUIVALENCE(TEM(1),      C(5)),      (TEM(4),      C(8))
        EQUIVALENCE(K,           C(9)),      (KK,          C(10))
        EQUIVALENCE(AMOL(1),     C(1171)),   (AMOL(1365),  C(2535))
        EQUIVALENCE(TITLE(1),    C(479)),    (TITLE(315),  C(793))
        EQUIVALENCE(IOMIT(1),    C(794)),    (IOMIT(105),  C(898))
        EQUIVALENCE(ILESS(1),    C(899)),    (ILESS(105),  C(1003))
        EQUIVALENCE(IN,          C(2539)),   (N,           C(2540))
        EQUIVALENCE(ME,          C(2542))
        DIMENSION AMOL(13,105),TITLE(3,105),IOMIT(105),ILESS(105)
        DIMENSION FMT(4),TEM(4)
SA      ALF    (1H+,
SB      ALF    A6,F8.
SC      ALF    5)
SD      ALF      7X,2
SE      ALF     36X,2
SF      ALF     64X,2
SG      ALF     92X,2
SOMIT   ALF    OMIT
      1 FORMAT (1X,2A6,2X,13F9.5)
      3 FORMAT (1H0,    118HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT W
       1HOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDI
       2TIONS//)
      4 FORMAT (1H0,     59HPRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM
       1CALCULATIONS//)
        TEM(1)=D
        TEM(2)=E
        TEM(3)=F
        TEM(4)=G
        FMT(1)=A
        FMT(3)=B
        FMT(4)=C
        K=0
        KK=4
        IOM=0
        ILE=0
        IF(ME-1)61,60,61
     61 WRITE OUTPUT TAPE 6,44
     60 II=0
        DO 9 I=1,N
S       CLA TITLE (1,I)
S       SUB OMIT
S       TNZ *10
```

```
      IOM=IOM+1
      IOMIT(IOM)=I
      GO TO 9
   10 DO 11 J=1,IN
      IF(AMOL(J,I)-.5E-05)11,12,12
   11 CONTINUE
      ILE=ILE+1
      ILESS(ILE)=I
      GO TO 9
   12 IF(ME-1)51,50,51
   50 WRITE OUTPUT TAPE 6,1 ,TITLE(2,I),TITLE(3,I),(AMOL(JJ,I),JJ=1,IN)
      GO TO 9
   51 II=II+1
      IF(II-KK)200,200,201
  200 K=K+1
      GO TO 5
  201 K=1
      KK=KK+4
      WRITE OUTPUT TAPE 6,44
   44 FORMAT (1H )
    5 FMT(2)=TEM(K)
      WRITE OUTPUT TAPE 6,FMT,TITLE(2,I),TITLE(3,I),AMOL(1,I)
    9 CONTINUE
      IF(ILE) 21,20,21
   21 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,3
      CALL ONCE (ILE,ILESS)
   20 IF(IOM) 31,30,31
   31 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,4
      CALL ONCE (IOM,IOMIT)
   30 RETURN
C
C
C
C
C
C
      SUBROUTINE PERPAR
C     OUTPUTS PERFORMANCE PARAMETERS
C
C
      COMMON C
      EQUIVALENCE(NN(1),       C(1)),      (NN(13),      C(13))
      EQUIVALENCE(PAR(1),      C(794)),    (PAR(208),    C(1001))
      EQUIVALENCE(IN,          C(2539)),   (MAY,         C(2543))
      EQUIVALENCE(KODE,        C(2544))
      DIMENSION PAR(13,16),NN(13)
   10 FORMAT (5H PC/P,10X)
   11 FORMAT (8H P, ATM ,7X)
   12 FORMAT (9H T, DEG K,6X,13I9)
   13 FORMAT (9H H, CAL/G,6X,13F9.1)
   14 FORMAT (15H S, CAL/(G)(K) 13F9.4)
   15 FORMAT (10H0M, MOL WT,5X,13F9.3)
   16 FORMAT (11H (DLM/DLP)T,4X,13F9.5)
   17 FORMAT (11H (DLM/DLT)P,4X,13F9.4)
   18 FORMAT (15H CP, CAL/(G)(K)13F9.4)
   19 FORMAT (6H GAMMA,9X,13F9.4)
   20 FORMAT (12H MACH NUMBER,3X,13F9.3)
   21 FORMAT (15H0CSTAR, FT/SEC 13I9)

   22 FORMAT (3H CF,12X,13F9.3)
   23 FORMAT (6H AE/AT,9X,13F9.3)
   24 FORMAT (15H IVAC,LB-SEC/LB13F9.1)
   25 FORMAT (15H I, LB-SEC/LB  13F9.1)
      IF(KODE-1)2,1,2
    1 WRITE OUTPUT TAPE 6,111
  111 FORMAT (8H0P, ATM ,7X)
      GO TO 3
    2 WRITE OUTPUT TAPE 6,10
      CALL VAR(1)
      WRITE OUTPUT TAPE 6,11
    3 CALL VAR(2)
      DO 60 I=1,IN
   60 NN(I)=PAR(I,3)+.5
      WRITE OUTPUT TAPE 6,12,(NN(I),I=1,IN)
      WRITE OUTPUT TAPE 6,13,(PAR(I,4),I=1,IN)
      WRITE OUTPUT TAPE 6,14,(PAR(I,5),I=1,IN)
      WRITE OUTPUT TAPE 6,15,(PAR(I,6),I=1,IN)
      IF(KODE)6,5,6
    6 WRITE OUTPUT TAPE 6,16,(PAR(I,8),I=1,IN)
      WRITE OUTPUT TAPE 6,17,(PAR(I,9),I=1,IN)
    5 WRITE OUTPUT TAPE 6,18,(PAR(I,7),I=1,IN)
      WRITE OUTPUT TAPE 6,19,(PAR(I,10),I=1,IN)
      IF(KODE-1)41,40,41
   40 RETURN
   41 WRITE OUTPUT TAPE 6,20,(PAR(I,12),I=1,IN)
      DO 61 I=1,IN
   61 NN(I)=PAR(I,15)+.5
      IF (MAY-1) 51,50,51
   50 WRITE OUTPUT TAPE 6,31,(NN(I),I=2,IN)
      WRITE OUTPUT TAPE 6,32,(PAR(I,16),I=2,IN)
      WRITE OUTPUT TAPE 6,33
      CALL VAR(11)
      WRITE OUTPUT TAPE 6,34,(PAR(I,14),I=2,IN)
      WRITE OUTPUT TAPE 6,35,(PAR(I,13),I=2,IN)
   31 FORMAT (15H0CSTAR, FT/SEC ,9X,12I9)
   32 FORMAT (3H CF,21X,12F9.3)
   33 FORMAT (6H AE/AT,18X,12F9.3)
   34 FORMAT (15H IVAC,LB-SEC/LB,9X,12F9.1)
   35 FORMAT (15H I, LB-SEC/LB ,9X,12F9.1)
      RETURN
   51 WRITE OUTPUT TAPE 6,21,(NN(I),I=1,IN)
      WRITE OUTPUT TAPE 6,22,(PAR(I,16),I=1,IN)
      WRITE OUTPUT TAPE 6,23
      CALL VAR(11)
      WRITE OUTPUT TAPE 6,24,(PAR(I,14),I=1,IN)
      WRITE OUTPUT TAPE 6,25,(PAR(I,13),I=1,IN)
      RETURN
C
C
C
      SUBROUTINE VAR(INDEX)
C     SPECIAL FORMAT FOR PC/P,P, AND AE/AT
C
C
      COMMON C
      EQUIVALENCE(TEMM(1),     C(1)),      (TEMM(13),    C(13))
      EQUIVALENCE(AM(1),       C(14)),     (AM(4),       C(17))
      EQUIVALENCE(TEM(1),      C(18)),     (TEM(4),      C(21))
      EQUIVALENCE(FMT(1),      C(22)),     (FMT(3),      C(24))
```

```
      EQUIVALENCE(PAR(1),      C(794)),   (PAR(208),    C(1001))
      EQUIVALENCE(IN,          C(2539)),  (MAY,         C(2543))
      DIMENSION FMT(3),PAR(13,16),TEM(4),AM(4),TEMM(13)
SA    ALF     14X,F
SB    ALF     23X,F
SC    ALF     32X,F
SD    ALF     41X,F
SE    ALF     50X,F
SF    ALF     59X,F
SAA   ALF     68X,F
SBB   ALF     77X,F
SCC   ALF     86X,F
SDD   ALF     95X,F
SEE   ALF    104X,F
SFF   ALF    113X,F
SGG   ALF    122X,F
SFOR  ALF    (1H+,
SZERO ALF    9.0)
SONE  ALF    9.1)
STWO  ALF    9.2)
STHR  ALF    9.3)
SFR   ALF    9.4)
      TEMM(1)=A
      TEMM(2)=B
      TEMM(3)=C
      TEMM(4)=D
      TEMM(5)=E
      TEMM(6)=F
      TEMM(7)=AA
      TEMM(8)=BB
      TEMM(9)=CC
      TEMM(10)=DD
      TEMM(11)=EE
      TEMM(12)=FF
      TEMM(13)=GG
      FMT(1)=FOR
      IF(INDEX-2) 1,2,3
    1 TEM(1)=1.0E04
      TEM(2)=1.0E05
      TEM(3)=1.0E06
      AM(1)=THR
      AM(2)=TWO
      AM(3)=ONE
      AM(4)=ZERO
      GO TO 4
    2 TEM(1)=1.0
      TEM(2)=10.0
      TEM(3)=100.0
      AM(1)=FR
      AM(2)=THR
      AM(3)=TWO
      AM(4)=ONE
      GO TO 4
    3 TEM(1)=10.0
      TEM(2)=100.0
      TEM(3)=1000.0
      AM(1)=THR
      AM(2)=TWO
      AM(3)=ONE
      AM(4)=ZERO

    4 DO 5 I=1,IN
      IF (I-1) 53,50,53
   50 IF (MAY-1) 53,52,53
   52 IF(INDEX-11) 53,5,53
   53 CONTINUE
      FMT(2)=TEMM(I)
      DO 6 J=1,3
      IF(PAR(I,INDEX)-TEM(J))10,6,6
   10 FMT(3)=AM(J)
   11 WRITE OUTPUT TAPE 6,FMT,PAR(I,INDEX)
      GO TO 5
    6 CONTINUE
      FMT(3)=AM(4)
      WRITE OUTPUT TAPE 6,FMT,PAR(I,INDEX)
    5 CONTINUE
      RETURN
```

APPENDIX D

PROGRAM LISTING FOR IBM 7090

```
C      MAIN PROGRAM
C
C
       COMMON C
       EQUIVALENCE   (G(1),        C(1)),    (G(420),      C(420))
       EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),      C(874))
       EQUIVALENCE   (HSUM,        C(424)),  (SSUM,        C(425))
       EQUIVALENCE   (WTMOL,       C(426)),  (CP,          C(427))
       EQUIVALENCE   (DLMPT,       C(428)),  (DLMTP,       C(429))
       EQUIVALENCE   (GAMMA,       C(430)),  (ARATIO,      C(431))
       EQUIVALENCE   (VMACH,       C(432)),  (SP IMP,      C(433))
       EQUIVALENCE   (VACI,        C(434)),  (CF,          C(436))
       EQUIVALENCE   (RHOI,        C(437)),  (RHOVAC,      C(438))
       EQUIVALENCE   (RHO,         C(439))
       EQUIVALENCE   (T PI,        C(440)),  (PI I,        C(441))
       EQUIVALENCE   (EP PI,       C(442)),  (AW PI,       C(443))
       EQUIVALENCE   (T ETA,       C(445))
       EQUIVALENCE   (ETA I,       C(446)),  (EP ETA,      C(447))
       EQUIVALENCE   (AW ETA,      C(448)),  (T SIG,       C(450))
       EQUIVALENCE   (SIG I,       C(451)),  (EP SIG,      C(452))
       EQUIVALENCE   (AW SIG,      C(453))
       EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
       EQUIVALENCE   (FORM(1),     C(1329)), (FORM(15),  C(1343))
       EQ'JIVALENCE  (ELMT(1),     C(1344)),  (ELMT(15), C(1358))
       EQUIVALENCE   (LLMT(1),     C(1344)),  (LLMT(15), C(1358))
       EQUIVALENCE   (DATA(1),   C(1359)),  (DATA(23),   C(1381))
       EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
       EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
       EQUIVALENCE   (ISYS,      C(1472)),    (JEAN,      C(1473))
       EQUIVALENCE   (ACX,       C(1474)),    (ACF,     C(1475))
       EQUIVALENCE   (AMX,        C(1476)),    (AMF,       C(1477))
       EQUIVALENCE   (RHOX,       C(1478)),    (RHOF,     C(1479))
       EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
       EQUIVALENCE   (DX(1),     C(1500)),  (DX(20),    C(1519))
       EQUIVALENCE   (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
       EQUIVALENCE   (MMLA(1),    C(1520)),  (MMLA(18), C(1537))
       EQUIVALENCE   (PROD(1),  C(1538)),  (PROD(3),    C(1540))
       EQUIVALENCE   (SYSTM(1),  C(1541)),  (SYSTM(15),   C(1555))
       EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
       EQUIVALENCE   (OF,     C(1556)),     (FPCT,   C(1557))
       EQUIVALENCE   (EQRAT,      C(1558))
       EQUIVALENCE (KODE,    C(1559)),   (KASE,      C(1560))
       EQUIVALENCE   (KONT,   C(1561)),   (NF,        C(1562))
       EQUIVALENCE   (NO,         C(1563)), (NE,        C(1564))
       EQUIVALENCE   (NOEQ, C(1565))
       EQUIVALENCE   (BOX(1),     C(1771)), (BOX(15),    C(1785))
       EQUIVALENCE   (BOF(1),     C(1786)), (BOF(15),    C(1800))
       EQUIVALENCE   (HX,         C(1801)), (HF,         C(1802))
       EQUIVALENCE   (VXPLS,      C(1803)), (VXMIN,      C(1804))
       EQUIVALENCE   (VFPLS,      C(1805)), (VFMIN,      C(1806))
       EQUIVALENCE   (EN LN(1),   C(1861)), (EN LN(90), C(1950))
       EQUIVALENCE   (DEL N(1),   C(1951)), (DEL N(90), C(2040))
       EQUIVALENCE   (H0(1),      C(2041)), (H0(90),     C(2130))
       EQUIVALENCE   (S(1),       C(2131)), (S(90),      C(2220))
       EQUIVALENCE   (X(1),       C(2221)), (X(20),      C(2240))
       EQUIVALENCE   (DELTA(1),   C(2241)), (DELTA(20), C(2260))
       EQUIVALENCE   (B0(1),      C(2261)), (B0(15),     C(2275))
       EQUIVALENCE   (P0,         C(2276)), (HSUB0,      C(2277))
       EQUIVALENCE   (S0,         C(2278)), (T LN,       C(2279))
       EQUIVALENCE   (T,          C(2280)), (AAY LN,     C(2281))

       EQUIVALENCE   (AAY,        C(2282)), (CPSUM,      C(2283))
       EQUIVALENCE   (HC,         C(2284)), (TC LN,      C(2285))
       EQUIVALENCE   (PCP(1),     C(2286)), (PCP(25),    C(2310))
       EQUIVALENCE   (DATUM(1),   C(2311)), (DATUM(3),   C(2313))
       EQUIVALENCE   (PC,         C(2314)), (TC,         C(2315))
       EQUIVALENCE   (IPROB,      C(2316)), (IFIXT,      C(2317))
       EQUIVALENCE   (IHS,        C(2318)), (ICOND,      C(2319))
       EQUIVALENCE   (ISYM,       C(2320)), (IPROD,      C(2321))
       EQUIVALENCE   (IDID,       C(2322)), (LDRUM,      C(2323))
       EQUIVALENCE   (IDRM,       C(2323)), (KDRUM,      C(2324))
       EQUIVALENCE   (L,          C(2325)), (L1,         C(2326))
       EQUIVALENCE   (M,          C(2327)), (M1,         C(2328))
       EQUIVALENCE   (N,          C(2329)), (IQ,         C(2330))
       EQUIVALENCE   (IQ1,        C(2331)), (IQ2,        C(2332))
       EQUIVALENCE   (IQ3,        C(2333)), (KMAT,       C(2334))
       EQUIVALENCE   (IMAT,       C(2335)), (IUSE,       C(2335))
       EQUIVALENCE   (IADD,       C(2336)), (ITNUMB,     C(2337))
       EQUIVALENCE   (ITAPE,      C(2338)), (P,          C(2339))
       EQUIVALENCE   (IDEBUG,     C(2340)), (IFROZ,      C(2341))
       EQUIVALENCE   (A(1),       C(2342)),  (A(1350),  C(3691))
       EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
       EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
       EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
       EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
       EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
       EQUIVALENCE (KORE, C(8047))
       EQUIVALENCE(MT,DMT)
       EQUIVALENCE (HS,MHS),(TS,MTS),(PT,MPT),(TP,MTP),(DET,MDET)
       EQUIVALENCE (PROB,MPROB),(END,MEND)
       EQUIVALENCE (TMLM,MTMLM) , (BLK,MBLK)
C
       DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
       DIMENSION   DEL N(90),  H0(90),     S(90),      X(20)
       DIMENSION   DELTA(20),  B0(15),     PCP(25),    PROD(3)
       DIMENSION   COEFX(20),  DX(20),     FORM(15)
       DIMENSION COEFT1(15,90) , COEFT2(15,90)
       DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
       DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
       DIMENSION LLMT(15),MTSYS(15),MDATA(23)
       DIMENSION   ANSLAB(454),   COEFT(15,90)
       DIMENSION   MATOM(101,3),      ATOM(101,3)
C
C
B1     H S=307362606060
B      T S=637362606060
B      P T=477363606060
B      T P=637347606060
B      DET=242563456060
B      END=254524606060
B      BLK=000000000060
B      OMIT=464431636060
B      DMT=606060606060
C
C
C      READ IN INPUT DATA
C
       IF (ISYS-99) 401,403,401
   403 READ TAPE 3,(G(I),I=1,8044)
       REWIND 3
       IF (SENSE SWITCH 6) 651,719
```

```
  401 ISYS=99
      IFROZ=0
      PAUSE 11111
  429 CALL INPUT
      IF (L) 651,651,433
  433 WRITE OUTPUT TAPE 6,443, HX,VXPLS,VXMIN,HF,VFPLS,VFMIN
     1, (ELMT(I),BOX(I),BOF(I),I=1,L)
  443 FORMAT (10H1OXIDANT  3E16.6/10H FUEL     3E16.6/(1H A6,2E20.8))
C
C     RIGHT ADJUST ELEMENT SYMBOLS
C
      DO 447 K=1,L
      TMLM = ELMT(K)
      ELMT(K) = ARSF(24, TMLM)
B     TMLM = ELMT(K) *0      00077
      IF (MTMLM-MBLK) 447,1447,447
 1447 TMLM = ELMT(K)
      ELMT(K) = ARSF(6, TMLM)
  447 CONTINUE
      IF(SYSTM(L+1))453,920,453
  920 IF (SYSTM(L)) 921,453,921
  921 DO 449 K=1,L
      DO 448 J=1,L
      IF (LLMT(K)-MTSYS(J)) 448,449,448
  448 CONTINUE
      GO TO 453
  449 CONTINUE
C
C     CANCEL ---OMITS---FROM PREVIOUS PROBLEM
C
  452 DO 1452 J=1,M
      COEFT1(1,J) = DMT
      COEFT2(1,J) = DMT
 1452 COEFT(1,J) = DMT
      IUSE=1
      GO TO 598
  453 DO 459 K=1,15
  459 SYSTM(K)=ELMT(K)
      CALL SEARCH
  598 IF (IUSE-2) 600,635,635
C
C     SET ARRAY  PROD  TO BY"ASS ALL CONDENSED PHASES
C
  600 PROD(1)=0.0
      PROD(2)=0.0
      IF (M-35) 198,198,1198
 1198 IF (M-70) 199,199,1199
 1199 IF (M-90) 200,200,635
B198  PROD(2)=377777777777
B     PROD(3) = 377777777777
      TMP=PROD(2)
      PROD(1)=ARSF(M,TMP)
      GO TO 201
  199 M12 = M-35
B     PROD(3) = 377777777777
      TMP=PROD(3)
      PROD(2)=ARSF(M12,TMP)
      GO TO 201
  200 M12 = M-70
B     PROD(3) = 377777777777

      TMP=PROD(3)
      PROD(3)=ARSF(M12,TMP)
  201 IQ=L
      IQ1=IQ+1
      IQ2=IQ1+1
      IQ3=IQ2+1
      L1=IQ1
      M1=M+1
C
C     DETERMINE WHICH GASEOUS SPECIES SHOULD BE OMITTED FROM THE PROBLEM
C     AND WHICH CONDENSED SPECIES SHOULD BE USED IN THE FIRST ITERATION
C
  203 READ INPUT TAPE 7,204,(DATA(I),I=1,8)
  204 FORMAT (4(2A6,3X))
B     SJW=DATA(1)*(-DMT)
B     IF(SJW)207,220,207
  207 DO 213 K=1,4
      DO 211 J=1,N
      DO 208 I=2,3
      KK=2*K+I-3
B     SJW=DATA(KK)*(-COEFT2(I,J))
B     IF(SJW)211,208,211
  208 CONTINUE
      IF (J-M) 209,209,210
  209 CALL BYPASS (J,2)
11209 GO TO 213
  210 CALL BYPASS (J,3)
11210 GO TO 213
  211 CONTINUE
  213 CONTINUE
      GO TO 203
  220 CONTINUE
      DO 222 J=1,M
      CALL BYPASS(J,1)
      IF (IPROD - 2) 221,222,221
  221 COEFT1(1,J) = OMIT
      COEFT2(1,J)=OMIT
  222 CONTINUE
C
C     ARRANGE ANSWER REGION
C
      I=1
      DO 602 J=1,N
      ANS(I)=COEFT2(1,J)
      ANS(I+1)=COEFT2(2,J)
      ANS(I+2)=COEFT2(3,J)
      ANS(I+3) = 0.0
  602 I=I+4
      K=4*N
  605 I=K+34
      ANS(I)=ANS(K)
      K=K-1
      IF (K) 651,607,605
  607 DO 609 K=1,34
  609 ANS(K) = 0.0
      DO 1700  K= 1, 454
 1700 ANSLAB(K) = ANS(K)
      DO 1701 J = 1, 15
      DO 1701 K = 1, 90
 1701 COEFT(J,K) = COEFT1(J,K)
```

```
C
C     DETERMINE THE TYPE OF PROBLEM
C
  700 IFROZ=1
  701 READ INPUT TAPE 7,703,PROB,KASE
  703 FORMAT (A5,I5)
      IF (MPROB-MHS) 705,901,705
  901 IPROB=1
      GO TO 715
  705 IF (MPROB-MTS) 707,902,707
  902 IPROB=2
      GO TO 715
  707 IF (MPROB-MPT) 709,903,709
  903 IPROB=3
      GO TO 715
  709 IF (MPROB-MTP) 711,904,711
  904 IPROB=4
      GO TO 715
  711 IF (MPROB-MDET) 713,905,713
  905 IPROB=1
      IFROZ=-1
      GO TO 719
  713 IF (MPROB-MT)631,429,631
  715 DO 716 K=1,25
  716 PCP(K)=0.0
      I=0
 1716 READ INPUT TAPE 7,718,(G(K),K=1,5)
      IF(G(1))719,719,717
  717 DO 1717 K=1,5
      IK=I+K
 1717 PCP(IK)=G(K)
      I=I+5
      GO TO 1716
  718 FORMAT(5F10.2)
C
C     DETERMINE THE ASSIGNED VALUES FOR THE PROBLEM
C
  719 READ INPUT TAPE 7,721,EQRAT,O F,F PCT,PC,TC,KODE,IDEBUG
  721 FORMAT (5F10.2,I5,16X,I1)
      IF (EQRAT) 725,725,723
  723 O F=(-EQRAT*VFMIN-VFPLS)/(VXPLS+EQRAT*VXMIN)
      F PCT=100.0/(1.0+O F)
      GO TO 745
  725 IF (O F) 731,731,727
  727 F PCT=100.0/(1.0+O F)
  729 EQRAT=ABSF((O F*VXPLS+VFPLS)/(O F*VXMIN+VFMIN))
      GO TO 745
  731 IF (F PCT) 700,700,733
  733 O F=(100.0-F PCT)/F PCT
      IF (O F)    719,1733,729
 1733 IF (VFMIN) 729, 746,729
  745 IF (O F) 719,746,746
  746 DO 747 I=1,L
  747 BO(I)=(O F*BOX(I)+BOF(I))/(1.0+O F)
      IF (IPROB-1) 651,749,748
  748 HSUBO=0.0
      GO TO 755
  749 HSUBO=(O F*HX+HF)/(1.0+O F)
  755 WRITE OUTPUT TAPE 6,760,KASE,PROB,O F,F PCT,EQRAT,PC,HSUBO,
     1 (BO(I),I=1,L)

  760 FORMAT (1H1I5,3X,A6/1H 4E17.8/(1H 7E17.8))
      HSUBO=HSUBO/1.98726
      DO 1771 I = 1, 454
 1771 ANS(I) = ANSLAB(I)
      RHO=RHOX+O F*RHOF
      IF (RHO) 772,772,771
  771 RHO=(1.0+O F)*RHOX*RHOF/RHO
  772 DO 1772 I = 1, 454
 1772 ANSLAB(I) = ANS(I)
  775 IF (IFROZ) 777,651,779
  777 CALL CORE4
      IF (KORE) 1,779,1
  779 CALL CORE2
      GO TO 1
C
C     ERROR PRINT OUT
C
  631 WRITE OUTPUT TAPE 6,633,PROB,KASE
  633 FORMAT (21H1THERE IS NO PROBLEM A6,2X,I5)
      GO TO 651
  635 WRITE OUTPUT TAPE 6,637
  637 FORMAT (47H1TROUBLE IN COMPILING MASTER THERMODYNAMIC TAPE)
      REWIND 4
  639 READ TAPE 4,(DATA(I),I=1,23)
      WRITE OUTPUT TAPE 6,640,(DATA(I),I=1,23)
  640 FORMAT (1H 3A6,2F10.1/(1H 2F8.1,7E14.6))
      IF (MDATA(1)-MEND) 639,900,639
  900 WRITE OUTPUT TAPE 6,643, ((COEFT1(K,J),K=1,14),J=1,N)
      WRITE OUTPUT TAPE 6,643, ((COEFT2(K,J),K=1,14),J=1,N)
  643 FORMAT (1H 3A6,2F15.2/2F8.1,7E12.4//)
  651 REWIND 4
      PAUSE 77777
```

```
      SUBROUTINE SEARCH
C
C
      COMMON C
      EQUIVALENCE   (G(1),        C(1)),     (G(420),     C(420))
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),     C(874))
      EQUIVALENCE   (HSUM,        C(424)),  (SSUM,        C(425))
      EQUIVALENCE   (WTMOL,       C(426)),  (CP,          C(427))
      EQUIVALENCE   (DLMPT,       C(428)),  (DLMTP,       C(429))
      EQUIVALENCE   (GAMMA,       C(430)),  (ARATIO,      C(431))
      EQUIVALENCE   (VMACH,       C(432)),  (SP IMP,      C(433))
      EQUIVALENCE   (VACI,        C(434)),  (CF,          C(436))
      EQUIVALENCE   (RHOI,        C(437)),  (RHOVAC,      C(438))
      EQUIVALENCE   (RHO,         C(439))
      EQUIVALENCE   (T PI,        C(440)),  (PI I,        C(441))
      EQUIVALENCE   (EP PI,       C(442)),  (AW PI,       C(443))
      EQUIVALENCE   (T ETA,       C(445))
      EQUIVALENCE   (ETA I,       C(446)),  (EP ETA,      C(447))
      EQUIVALENCE   (AW ETA,      C(448)),  (T SIG,       C(450))
      EQUIVALENCE   (SIG I,       C(451)),  (EP SIG,      C(452))
      EQUIVALENCE   (AW SIG,      C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),     C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (ELMT(1),     C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE   (LLMT(1),     C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE   (DATA(1),   C(1359)),   (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1!,   C(1359)),   (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),    C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,      C(1472)),    (JEAN,      C(1473))
      EQUIVALENCE   (ACX,       C(1474)),    (ACF,     C(1475))
      EQUIVALENCE   (AMX,         C(1476)),    (AMF,       C(1477))
      EQUIVALENCE   (RHOX,        C(1478)),    (RHOF,      C(1479))
      EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),     C(1500)),  (DX(20),    C(1519))
      EQUIVALENCE   (FORMLA(1), C(1520)),   (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),     C(1520)),   (MMLA(18), C(1537))
      EQUIVALENCE   (PROD(1),   C(1538)),   (PROD(3),    C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),   (SYSTM(15),   C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,      C(1556)),     (FPCT,   C(1557))
      EQUIVALENCE   (EQRAT,       C(1558))
      EQUIVALENCE (KODE,     C(1559)),    (KASE,       C(1560))
      EQUIVALENCE   (KONT,   C(1561)),     (NF,         C(1562))
      EQUIVALENCE   (NO,          C(1563)), (NE,         C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (BOX(1),      C(1771)), (BOX(15),    C(1785))
      EQUIVALENCE   (BOF(1),      C(1786)), (BOF(15),    C(1800))
      EQUIVALENCE   (HX,          C(1801)), (HF,         C(1802))
      EQUIVALENCE   (VXPLS,       C(1803)), (VXMIN,      C(1804))
      EQUIVALENCE   (VFPLS,       C(1805)), (VFMIN,      C(1806))
      EQUIVALENCE   (EN LN(1),    C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),    C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (H0(1),       C(2041)), (H0(90),     C(2130))
      EQUIVALENCE   (S(1),        C(2131)), (S(90),      C(2220))
      EQUIVALENCE   (X(1),        C(2221)), (X(20),      C(2240))
      EQUIVALENCE   (DELTA(1),    C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (B0(1),       C(2261)), (B0(15),     C(2275))
      EQUIVALENCE   (P0,          C(2276)), (HSUB0,      C(2277))
      EQUIVALENCE   (S0,          C(2278)), (T LN,       C(2279))
      EQUIVALENCE   (T,           C(2280)), (AAY LN,     C(2281))

      EQUIVALENCE   (AAY,         C(2282)), (CPSUM,      C(2283))
      EQUIVALENCE   (HC,          C(2284)), (TC LN,      C(2285))
      EQUIVALENCE   (PCP(1),      C(2286)), (PCP(25),    C(2310))
      EQUIVALENCE   (DATUM(1),    C(2311)), (DATUM(3),   C(2313))
      EQUIVALENCE   (PC,          C(2314)), (TC,         C(2315))
      EQUIVALENCE   (IPROB,       C(2316)), (IFIXT,      C(2317))
      EQUIVALENCE   (IHS,         C(2318)), (ICOND,      C(2319))
      EQUIVALENCE   (ISYM,        C(2320)), (IPROD,      C(2321))
      EQUIVALENCE   (IDID,        C(2322)), (LDRUM,      C(2323))
      EQUIVALENCE   (IDRM,        C(2323)), (KDRUM,      C(2324))
      EQUIVALENCE   (L,           C(2325)), (L1,         C(2326))
      EQUIVALENCE   (M,           C(2327)), (M1,         C(2328))
      EQUIVALENCE   (N,           C(2329)), (IQ,         C(2330))
      EQUIVALENCE   (IQ1,         C(2331)), (IQ2,        C(2332))
      EQUIVALENCE   (IQ3,         C(2333)), (KMAT,       C(2334))
      EQUIVALENCE   (IMAT,        C(2335)), (IUSE,       C(2335))
      EQUIVALENCE   (IADD,        C(2336)), (ITNUMB,     C(2337))
      EQUIVALENCE   (ITAPE,       C(2338)), (P,          C(2339))
      EQUIVALENCE   (IDEBUG,      C(2340)), (IFROZ,      C(2341))
      EQUIVALENCE   (A(1),        C(2342)),  (A(1350),  C(3691))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
      EQUIVALENCE (C12,MM),(E,ME),(END,MEND),(BLK,MBLK),(RPN,MRPN)
      EQUIVALENCE (GAS,MGAS),(SOL,MSOL),(BLIQ,MLIQ),(BLPN,MLPN)
      EQUIVALENCE (C10,MC10),(PLS,MPLS),(SYMBL,MBL),(BMIN,MMIN)
      EQUIVALENCE (TMP1, MTMP1)
C
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),      EN LN(90)
      DIMENSION   DEL N(90),  H0(90),     S(90),       X(20)
      DIMENSION   DELTA(20),  B0(15),     PCP(25),     PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),    FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),    SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),     ATOM(101,3)
      DIMENSION MMLA(18)
C
C
B     BLK=000000000060
B     RPN=000000000034
B     BLPN=000000000074
B     GAS=000000000027
B     SOL=000000000062
B     BLIQ=000000000043
B     PLS=000000000020
B     BMIN=000000000040
B     E=000000000025
B     END=254524606060
B     C10=000000000012
B     C12=000014000000
B     CF10=000012000000
C
C
      KION=2
```

```
      DO 1 K=1,L
      IF (LLMT(K)-ME) 1,2,1
    1 CONTINUE
      GO TO 3
    2 KION=1
      TEMP=ELMT(K)
      ELMT(K)=ELMT(L)
      ELMT(L)=TEMP
    3 ISOL=0
      M=0
      DO 4 J=1,15
      DO 4 K=1,90
      COEFT2(J,K) = 0.0
    4 COEFT1(J,K) = 0.0
      DO 6 J=1,1350
    6 A(J) = 0.0
      REWIND 4
    7 READ TAPE 4, (DATA(I),I=1,23)
      IF (MDATA(1)-MEND) 900,171,900
C
C     UNPACK THE BCD FORMULA FOR THE PRODUCT
C
  900 DO 16 I=1,2
   16 DATUM(I)=DATA(I)
      J=1
      I=1
   13 K=0
   17 TMP1 = DATUM(I)
      FORMLA(J) = ARSF(30,TMP1)
B     DATUM(I) ='ALSF(6       ,TMP1)
      J=J+1
      IF (K-4) 925,925,21
  925 K = K+1
      GO TO 17
   21 IF(I-1) 926,926,25
  926 I=I+1
      GO TO 13
C
C     BEGIN SEARCH FOR FIRST NON BLANK ALPHANUMERIC CHARACTER
C
   25 J=12
   29 J=J
      IF (MMLA(J)-MBLK) 35,950,35
  950 IF (J-1) 30,30,951
  951 J = J-1
      GO TO 29
   30 WRITE OUTPUT TAPE 6,31,(DATA(I),I=1,3)
   31 FORMAT (14H THE FORMULA  3A6,33H  IS INCORRECT ON THE MASTER TAPE)
      GO TO 7
   35 IF (MMLA(J)-MRPN) 30,952,30
  952 J = J-1
      IF (MMLA(J)-MGAS) 953,39,953
  953 IF (MMLA(J)-MSOL) 954,41,954
  954 IF (MMLA(J)-MLIQ) 30,41,30
   39 ITYPE=1
      GO TO 47
   41 ITYPE=2
   47 J=J-1
      IF (MMLA(J)-MLPN) 30,955,30
  955 J=J-1

C
C     OBTAIN AND STORE THE FORMULA NUMBERS A(K,J)
C
      DO 48 K=1,15
   48 FORM(K)=0.0
   51 NLSW=1
      NUMB=0
   55 ICNT=0
   57 JCNT=J-ICNT
      IF (JCNT) 30,81,59
   59 IF (MMLA(JCNT) - MC10) 958,67,67
  958 GO TO (63,85),NLSW
   63 ICNT=ICNT+1
      GO TO 57
   67 GO TO (69,63),NLSW
   69 IF (ICNT) 959,330,959
  330 IF(KION-1)30,333,30
  333 NLSW=2
      GO TO 57
  959 IF (ICNT-2) 77,73,30
   73 NUMB = MMLA(J-1) * 10
   77 TMP1 = FORMLA(J)
      TMP1 = ALSF(18,TMP1)
B     TMP1 = TMP1 * 377777777777
B     TMP2 = FORMLA(J) * 4000
B     TMP1 = TMP1 + TMP2
      NUMB = NUMB+ MTMP1
      VALUE=NUMB
      J=J-ICNT
      NLSW=2
      GO TO 55
   81 GO TO (30,85),NLSW
   85 IF (ICNT) 960,30,960
  960 SYMBL = 0.0
      IF(NUMB)86,95,86
   86 IF (ICNT-2) 93,89,30
   89 TMP1 = FORMLA(J-1)
      SYMBL = ALSF(6,TMP1)
   93 MBL = MBL + MMLA(J)
      GO TO 107
   95 IF(JCNT)30,30,96
   96 IF (MMLA(J)-MPLS) 97,970,97
  970 FORM(L)=-ICNT
      GO TO 109
   97 IF (MMLA(J)-MMIN) 107,975,107
  975 FORM(L)=ICNT
  101 GO TO 109
  107 DO 111 K=1,L
      IF (MBL-LLMT(K)) 111,105,111
  111 CONTINUE
      GO TO 7
  105 FORM(K)=VALUE
  109 J=J-ICNT
      IF (J) 30,121,51
  121 IF (ITYPE-1) 30,133,137
  133 M=M+1
      J=M
      GO TO 145
  137 J=90-ISOL
      ISOL=ISOL+1
```

```
  145 DO 147 K=1,L
      A(K,J)=FORM(K)
  147 CONTINUE
C
C     ARRANGE THERMODYNAMIC DATA IN CORE ORDERED BY INTERVAL
C
  151 IT=0
      TEMP = DATA(1)
      DATA(1) = DATA(3)
      DATA(3) = DATA(2)
      DATA(2) = TEMP
      DO 155 K=1,5
  155 COEFT1(K,J) = DATA(K)
      DO 159 K=6,14
      KIT= K+IT
  159 COEFT1(K,J) = DATA(KIT)
      IT=IT+9
      DO1955 K=1,5
 1955 COEFT2(K,J) = DATA(K)
      DO1959 K=6,14
      KIT = K+IT
 1959 COEFT2(K,J) = DATA(KIT)
      GO TO 7
C
C     GO TO NEXT MOLECULE
C
C
C     ELIMINATE GAP BETWEEN GASES AND CONDENSED PHASES
C
  171 N=M+ISOL
      IUSE=1
  173 IF (N-90) 175,225,181
  175 IF (ISOL) 177,225,184
  177 IUSE=2
      GO TO 225
  181 WRITE OUTPUT TAPE 6,182
  182 FORMAT (45H TOO MANY REACTION PRODUCTS FOUND ON THE TAPE)
      IUSE=2
      GO TO 225
  184 KK = 90-ISOL
      DO 186 J = 1, ISOL
      MJ = M+J
      KJ = KK + J
      DO 186 K = 1,15
  186 COEFT1(K,MJ) = COEFT1(K,KJ)
      DO 185 J = 1,ISOL
      MJ = M+J
      KJ = KK + J
      DO 185 K = 1,15
  185 COEFT2(K,MJ) = COEFT2(K,KJ)
      DO 219 J=1,ISOL
      MJ=M+J
      KJ = KK +J
      DO 217 K=1,15
      A(K,MJ) = A(K,KJ)
  217 CONTINUE
  219 CONTINUE
      GO TO 225
  225 RETURN
```

```
      SUBROUTINE BYPASS (J,IARG)
C
C
      COMMON C
      EQUIVALENCE   (G(1),      C(1)),     (G(420),     C(420))
      EQUIVALENCE   (ANS(1),  C(421)),   (ANS(454),     C(874))
      EQUIVALENCE   (HSUM,      C(424)),   (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,     C(426)),   (CP,         C(427))
      EQUIVALENCE   (DLMPT,     C(428)),   (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,     C(430)),   (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,     C(432)),   (SP IMP,     C(433))
      EQ'JIVALENCE  (VAC1,      C(434)),   (CF,         C(436))
      EQUIVALENCE   (RHOI,      C(437)),   (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,       C(439))
      EQUIVALENCE   (T PI,      C(440)),   (PI I,       C(441))
      EQUIVALENCE   (EP PI,     C(442)),   (AW PI,      C(443))
      EQUIVALENCE   (T ETA,     C(445))
      EQUIVALENCE   (ETA I,     C(446)),   (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,    C(448)),   (T SIG,      C(450))
      EQUIVALENCE   (SIG I,     C(451)),   (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,    C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),    C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (ELMT(1),    C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE   (LLMT(1),    C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE   (DATA(1),  C(1359)),   (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),   (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,     C(1472)),    (JEAN,     C(1473))
      EQUIVALENCE   (ACX,      C(1474)),    (ACF,     C(1475))
      EQUIVALENCE   (AMX,       C(1476)),    (AMF,      C(1477))
      EQUIVALENCE   (RHOX,      C(1478)),    (RHOF,     C(1479))
      EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),     C(1500)),  (DX(20),    C(1519))
      EQUIVALENCE   (FORMLA(1),  C(1520)),   (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),   C(1520)),   (MMLA(18), C(1537))
      EQUIVALENCE   (PROD(1),  C(1538)),   (PROD(3),    C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),   (SYSTM(15),    C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,      C(1556)),      (FPCT,   C(1557))
      EQUIVALENCE   (EQRAT,       C(1558))
      EQUIVALENCE (KODE,     C(1559)),     (KASE,       C(1560))
      EQUIVALENCE   (KONT,   C(1561)),    (NF,          C(1562))
      EQUIVALENCE   (NO,          C(1563)), (NE,        C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (BOX(1),      C(1771)), (BOX(15),   C(17ė5))
      EQUIVALENCE   (BOF(1),      C(1786)), (BOF(15),   C(1800))
      EQUIVALENCE   (HX,          C(1801)), (HF,        C(1802))
      EQUIVALENCE   (VXPLS,       C(1803)), (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,       C(1805)), (VFMIN,     C(1806))
      EQ'JIVALENCE  (EN LN(1),    C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),    C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (H0(1),       C(2041)), (H0(90),    C(2130))
      EQUIVALENCE   (S(1),        C(2131)), (S(90),     C(2220))
      EQUIVALENCE   (X(1),        C(2221)), (X(20),     C(2240))
      EQUIVALENCE   (DELTA(1),    C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (B0(1),       C(2261)), (B0(15),    C(2275))
      EQUIVALENCE   (P0,          C(2276)), (HSUB0,     C(2277))
      EQUIVALENCE   (S0,          C(2278)), (T LN,      C(2279))
      EQUIVALENCE   (T,           C(2280)), (AAY LN,    C(2281))

      EQUIVALENCE   (AAY,         C(2282)), (CPSUM,     C(2283))
      EQUIVALENCE   (HC,          C(2284)), (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),      C(2286)), (PCP(25),   C(2310))
      EQUIVALENCE   (DATUM(1),    C(2311)), (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,          C(2314)), (TC,        C(2315))
      EQUIVALENCE   (IPROB,       C(2316)), (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,         C(2318)), (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,        C(2320)), (IPROD,     C(2321))
      EQUIVALENCE   (IDID,        C(2322)), (LDRUM,     C(2323))
      EQUIVALENCE   (IDRM,        C(2323)), (KDRUM,     C(2324))
      EQUIVALENCE   (L,           C(2325)), (L1,        C(2326))
      EQUIVALENCE   (M,           C(2327)), (M1,        C(2328))
      EQUIVALENCE   (N,           C(2329)), (IQ,        C(2330))
      EQUIVALENCE   (IQ1,         C(2331)), (IQ2,       C(2332))
      EQUIVALENCE   (IQ3,         C(2333)), (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,        C(2335)), (IUSE,      C(2335))
      EQUIVALENCE   (IADD,        C(2336)), (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,       C(2338)), (P,         C(2339))
      EQUIVALENCE   (IDEBUG,      C(2340)), (IFROZ,     C(2341))
      EQUIVALENCE   (A(1),        C(2342)),  (A(1350),  C(3691))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQ'JIVALENCE  (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
      EQUIVALENCE (CONS,JFCONS),    (MTEMP, TEMP)
C
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  H0(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  B0(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),      ATOM(101,3)
C
C
C     IARG=1 MEANS TEST ONLY, IARG=2 MEANS ELIMINATE A SPECIES, IARG=3
C     MEANS ADD ANOTHER SPECIES
C
B     CONS=1
      MLM=J
      IF (J-35) 2,2,102
  102 IF (J-70) 1,1,101
  101 K=3
      MLM=J-70
      GO TO 3
    1 K=2
      MLM=J-35
      GO TO 3
    2 K=1
    3 IF (IARG-2) 4,5,7
    4 IPROD=2
      KLM = 35-MLM
      TEMP = PROD(K)
      TEMP = LRSF(KLM,TEMP)
B     IF (TEMP*CONS) 12,10,12
```

```
   12 IPROD = 1
      GO TO 10
    5 KLM = 35 - MLM
      TEMP = PROD(K)
      TEMP = LRSF(KLM,TEMP)
B     IF (TEMP * CONS) 10,6,1
B6    TEMP = TEMP +1
B     PROD(K) = LLSF(KLM,TEMP)
      IF(M-J)11,10,10
   11 IQ3=IQ2
      IQ2=IQ1
      IQ1=IQ
      IQ =IQ-1
      GO TO 9
    7 KLM = 35 - MLM
      TEMP = PROD(K)
      TEMP = LRSF(KLM,TEMP)
B     IF (TEMP * 1) 110,10,11
  110 MTEMP=MTEMP-JFCONS
B     PROD(K) = LLSF(KLM, TEMP)
      IF(M-J)121,10,10
  121 IQ = IQ1
      IQ1=IQ2
      IQ2=IQ3
      IQ3=IQ3+1
    9 SENSE LIGHT 4
   10 RETURN
```

```
      SUBROUTINE INPUT
C
C
      COMMON C
      EQUIVALENCE   (G(1),       C(1)),    (G(420),     C(420))
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),    C(874))
      EQUIVALENCE   (HSUM,       C(424)),  (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,      C(426)),  (CP,         C(427))
      EQUIVALENCE   (DLMPT,      C(428)),  (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,      C(430)),  (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,      C(432)),  (SP IMP,     C(433))
      EQUIVALENCE   (VACI,       C(434)),  (CF,         C(436))
      EQUIVALENCE   (RHOI,       C(437)),  (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),  (PI I,       C(441))
      EQUIVALENCE   (EP PI,      C(442)),  (AW PI,      C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),  (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,     C(448)),  (T SIG,      C(450))
      EQUIVALENCE   (SIG I,      C(451)),  (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),    C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (ELMT(1),    C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE   (LLMT(1),    C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE   (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,     C(1472)),   (JEAN,      C(1473))
      EQ'JIVALENCE  (ACX,      C(1474)),   (ACF,     C(1475))
      EQUIVALENCE   (AMX,        C(1476)),   (AMF,      C(1477))
      EQUIVALENCE   (RHOX,       C(1478)),   (RHOF,     C(1479))
      EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),    C(1500)),  (DX(20),   C(1519))
      EQUIVALENCE   (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),    C(1520)),  (MMLA(18), C(1537))
      EQUIVALENCE   (PROD(1),  C(1538)),  (PROD(3),    C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),  (SYSTM(15),   C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,     C(1556)),     (FPCT,   C(1557))
      EQUIVALENCE   (EQRAT,      C(1558))
      EQUIVALENCE (KODE,     C(1559)),    (KASE,      C(1560))
      EQUIVALENCE   (KONT,   C(1561)),    (NF,          C(1562))
      EQUIVALENCE   (NO,         C(1563)), (NE,         C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE (KD, C(1763))
      EQUIVALENCE   (BOX(1),     C(1771)), (BOX(15),    C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)), (BOF(15),    C(1800))
      EQUIVALENCE   (HX,         C(1801)), (HF,         C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)), (VXMIN,      C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)), (VFMIN,      C(1806))
      EQUIVALENCE (TELMT(1), C(1807)), (TELMT(15), C(1821))
      EQUIVALENCE   (EN LN(1),   C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (H0(1),      C(2041)), (H0(90),     C(2130))
      EQUIVALENCE   (S(1),       C(2131)), (S(90),      C(2220))
      EQUIVALENCE   (X(1),       C(2221)), (X(20),      C(2240))
      EQUIVALENCE   (DELTA(1),   C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (B0(1),      C(2261)), (B0(15),     C(2275))
      EQUIVALENCE   (P0,         C(2276)), (HSUB0,      C(2277))

      EQUIVALENCE   (S0,         C(2278)), (T LN,       C(2279))
      EQUIVALENCE   (T,          C(2280)), (AAY LN,     C(2281))
      EQUIVALENCE   (AAY,        C(2282)), (CPSUM,      C(2283))
      EQUIVALENCE   (HC,         C(2284)), (TC LN,      C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)), (PCP(25),    C(2310))
      EQUIVALENCE   (DATUM(1),   C(2311)), (DATUM(3),   C(2313))
      EQUIVALENCE   (PC,         C(2314)), (TC,         C(2315))
      EQUIVALENCE   (IPROB,      C(2316)), (IFIXT,      C(2317))
      EQUIVALENCE   (IHS,        C(2318)), (ICOND,      C(2319))
      EQUIVALENCE   (ISYM,       C(2320)), (IPROD,      C(2321))
      EQUIVALENCE   (IDID,       C(2322)), (LDRUM,      C(2323))
      EQUIVALENCE   (IDRM,       C(2323)), (KDRUM,      C(2324))
      EQUIVALENCE   (L,          C(2325)), (L1,         C(2326))
      EQUIVALENCE   (M,          C(2327)), (M1,         C(2328))
      EQUIVALENCE   (N,          C(2329)), (IQ,         C(2330))
      EQUIVALENCE   (IQ1,        C(2331)), (IQ2,        C(2332))
      EQUIVALENCE   (IQ3,        C(2333)), (KMAT,       C(2334))
      EQUIVALENCE   (IMAT,       C(2335)), (IUSE,       C(2335))
      EQUIVALENCE   (IADD,       C(2336)), (ITNUMB,     C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)), (P,          C(2339))
      EQ'JIVALENCE  (IDEBUG,     C(2340)), (IFROZ,      C(2341))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
      EQUIVALENCE(A(1), C(8578)),  (A(690), C(9267))
      EQUIVALENCE (MANAME(1),ANAME(1)),(MANAME(5),ANAME(5))
C
      DIMENSION TELMT(15)
      DIMENSION   G(20,21),   A(15,46),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  H0(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  B0(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),  COEFT(15,90)
      DIMENSION   MATOM(101,3),     ATOM(101,3)
      DIMENSION MANAME(5),     ANAME(5),      ANUM(5)
C
C
C    SUBROUTINE TO COMPUTE PROPELLANTS
B     OX=466060606060
      IF(JEAN-222)51,50,51
   51 CALL BCREAD(ATOM(101,3),ATOM(1,1))
   50 DO 52 I=1,15
B     ELMT(I)=000000000
B     BOF(I)=0000000000
B     BOX(I)=0000000000
      DO 52 J=1,46
B     A(I,J)=0000000000
   52 CONTINUE
      TOTAL=0.0
      NF=0
      NO=0
      NE=0
      WRITE OUTPUT TAPE 6,400
  400 FO?MAT(8H1  INPUT//)
```

```
100 READ INPUT TAPE 7,1,(ANAME(I),ANUM(I),I=1,5),PECWT,ENTH,
   2DEN,TEMP,ETHR,DENS
  1 FORMAT(5(A2,F7.5),F8.5,F9.5,A1,F8.5,A1,F8.5)
    IF(ANUM(1))99,200,99
 99 WRITE OUTPUT TAPE 6,402,(ANAME(I),ANUM(I),I=1,5),PECWT,ENTH,DEN,
   2TEMP,ETHR,DENS
402 FORMAT (1X,5(A2,1X,F7.4,2X),F8.4,2X,F9.2,2X,A1,2X,F8.3,2X,
   2A1,3X,F8.5)
    DO 9 I=1,5
  9 TOTAL=TOTAL+ANUM(I)
    IF(ETHR-OX)11,10,11
 10 NO=NO+1
    KK=NO
    KKK=NO
    NN=31
    GO TO 12
 11 NF=NF+1
    KK=NF+15
    KKK=NF
    NN=32
 12 DO 98 J=1,5
    IF(ANUM(J)) 96,97,96
 96 DO 31 I=1,15
    IF(ANAME(J)-ELMT(I)) 21,20,21
 20 NHUT=0
 33 KT=I
    GO TO 30
 21 IF(ELMT(I)) 31,22,31
 22 ELMT(I)=ANAME(J)
    NE=NE+1
    NHUT=1
    GO TO 33
 31 CONTINUE
 30 IF(NHUT)14,15,14
 14 DO 16 I=1,101
    IF (MATOM(I,1)-MANAME(J)) 16,17,16
 17 II=I
    GO TO 18
 16 CONTINUE
    WRITE OUTPUT TAPE 6,199
199 FORMAT (32H0 THERE IS A BAD PROPELLANT CARD)
    L=-1
    RETURN
 18 A(NE,37)=ATOM(II,2)
    A(NE,38)=ATOM(II,3)
 15 A(KT,KK)=ANUM(J)
 98 CONTINUE
 97 A(KKK,NN)=ENTH
    A(KKK,NN+2)=PECWT
    A(KKK,NN+4)=DENS
    A(KKK,NN+10)=DEN
    A(KKK,NN+12)=TEMP
    A(KKK,NN+14)=ETHR
    GO TO 100
200 IF(NE)202,201,202
201 L=0
    RETURN
202 JEAN=222
B       WX=00000000000
B       WF=00000000000

B       HX=00000000000
B       HF=00000000000
B       RHOX=00000000000
B       RHOF=00000000000
B       VXPLS=0000000000
B       VXMIN=0000000000
B       VFPLS=0000000000
B       VFMIN=0000000000
B       ACX=00000000000
B       ACF=00000000000
B       AMX=00000000000
B       AMF=00000000000
    DO552 J=1,NO
    DO552 I=1,NE
552 A(J,39)=A(J,39)+A(I ,37)*A(I ,J )
    DO 53 J=1,NF
    DO 53 I=1,NE
 53 A(J,40)=A(J,40)+A(I,37)*A(I,J+15)
    IF (NO) 1000,1001,1000
1000 DO 550 I=1,NO
 54 HX=HX+A(I,31)*A(I,33)/A(I,39)
550 WX=WX+A(I,33)
1001 IF (NF) 1002,1003,1002
1002 DO 551 I=1,NF
 55 HF=HF+A(I,32)*A(I,34)/A(I,40)
551 WF=WF+A(I,34)
1003 IF (NO) 1004,1005,1004
1004 DO 42 I=1,NO
    ACX=ACX+A(I,35)*A(I,33)/A(I,39)
 42 AMX=AMX+A(I,33)/A(I,39)
    ACX=ACX/WX
    AMX=WX/AMX
1005 IF (NF) 1006,1007,1006
1006 DO 43 I=1,NF
    ACF=ACF+A(I,36)*A(I,34)/A(I,40)
 43 AMF=AMF+A(I,34)/A(I,40)
    ACF=ACF/WF
    AMF=WF/AMF
1007 IF (WX) 1020,1021,1020
1020 HX=HX/WX
1021 IF (WF) 1022,1023,1022
1022 HF =HF/WF
1023 DO 60 I=1,NO
    IF(A(I,35))60,71,60
 60 RHOX=RHOX+A(I,33)/A(I,35)
    RHOX=WX/RHOX
 73 DO 61 I=1,NF
    IF(A(I,36))61,71,61
 61 RHOF=RHOF+A(I,34)/A(I,36)
    RHOF=WF/RHOF
    GO TO 74
 71 RHOX = 0.0
 72 RHOF = 0.0
 74 IF (NO) 1008,1009,1008
1008 DO 57 I=1,NE
    DO 56 J=1,NO
 56 BOX(I)=BOX(I)+A(I,J)*A(J,33)/A(J,39)
 57 BOX(I)=BOX(I)/WX
1009 IF (NF) 1010,1011,1010
1010 DO 59 I=1,NE
```

```
      DO 58 J=1,NF
   58 BOF(I)=BOF(I)+A(I,J+15)*A(J,34)/A(J,40)
   59 BOF(I)=BOF(I)/WF
 1011 DO 62 I=1,NE
      IF(A(I,38))63,62,64
   64 VXPLS=VXPLS+BOX(I)*A(I,38)
   67 VFPLS=VFPLS+BOF(I)*A(I,38)
      GO TO 62
   63 VXMIN=VXMIN+BOX(I)*A(I,38)
   66 VFMIN=VFMIN+BOF(I)*A(I,38)
   62 CONTINUE
      IF (WX) 1030,1031,1030
 1030 DO 40 I=1,NO
   40 A(I,33)=A(I,33)/WX
 1031 IF (WF) 1040,1041,1040                     — see errata
 1040 DO 1041 I= 1,NF
 1041 A(I,34)=A(I,34)/WF
C
C     SAVE ELEMENT ARRAY FOR CORE 4
C
      DO 2000 I= 1,15                            — see errata
 2000 TELMT(I) = ELMT(I)
      L=NE
      TOTAL = MODF(TOTAL,1.0)
      IF(TOTAL)1142,1143,1142
 1142 KD=1
      RETURN
 1143 KD=0
      RETURN
```

```
      SUBROUTINE  CORE2
C
      COMMON C
      EQUIVALENCE   (G(1),       C(1)),    (G(420),     C(420))
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),     C(874))
      EQUIVALENCE   (HSUM,       C(424)),  (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,      C(426)),  (CP,         C(427))
      EQUIVALENCE   (DLMPT,      C(428)),  (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,      C(430)),  (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,      C(432)),  (SP IMP,     C(433))
      EQUIVALENCE   (VACI,       C(434)),  (CF,         C(436))
      EQUIVALENCE   (RHOI,       C(437)),  (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,        C(439))
      EQUIVALENCE   (T PI,       C(440)),  (PI I,       C(441))
      EQUIVALENCE   (EP PI,      C(442)),  (AW PI,      C(443))
      EQUIVALENCE   (T ETA,      C(445))
      EQUIVALENCE   (ETA I,      C(446)),  (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,     C(448)),  (T SIG,      C(450))
      EQUIVALENCE   (SIG I,      C(451)),  (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,     C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),    C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (MFORM(1),   C(1329)), (MFORM(15), C(1343))
      EQUIVALENCE   (ELMT(1),    C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE   (LLMT(1),    C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE   (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,     C(1472)),   (JEAN,     C(1473))
      EQUIVALENCE   (ACX,      C(1474)),   (ACF,     C(1475))
      EQUIVALENCE   (AMX,        C(1476)),   (AMF,      C(1477))
      EQUIVALENCE   (RHOX,       C(1478)),   (RHOF,    C(1479))
      EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),    C(1500)),  (DX(20),   C(1519))
      EQUIVALENCE   (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),    C(1520)),  (MMLA(18), C(1537))
      EQUIVALENCE   (SYSTM(1),   C(1541)),  (SYSTM(15),   C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,      C(1556)),     (FPCT,   C(1557))
      EQUIVALENCE   (EQRAT,      C(1558))
      EQUIVALENCE (KODE,     C(1559)),   (KASE,       C(1560))
      EQUIVALENCE   (KONT,   C(1561)),   (NF,           C(1562))
      EQUIVALENCE   (NO,         C(1563)), (NE,         C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (BOX(1),     C(1771)), (BOX(15),    C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)), (BOF(15),    C(1800))
      EQUIVALENCE   (HX,         C(1801)), (HF,         C(1802))
      EQUIVALENCE   (VXPLS,      C(1803)), (VXMIN,      C(1804))
      EQUIVALENCE   (VFPLS,      C(1805)), (VFMIN,      C(1806))
      EQUIVALENCE   (EN LN(1),   C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),   C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (HO(1),      C(2041)), (HO(90),     C(2130))
      EQUIVALENCE   (S(1),       C(2131)), (S(90),      C(2220))
      EQUIVALENCE   (MX(1),    C(2221)), (MX(20),     C(2240))
      EQUIVALENCE   (X(1),       C(2221)), (X(20),      C(2240))
      EQUIVALENCE   (DELTA(1),   C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (BO(1),      C(2261)), (BO(15),     C(2275))
      EQUIVALENCE   (PO,         C(2276)), (HSUBO,      C(2277))
      EQUIVALENCE   (SO,         C(2278)), (T LN,       C(2279))
      EQUIVALENCE   (T,          C(2280)), (AAY LN,     C(2281))

      EQUIVALENCE   (AAY,        C(2282)), (CPSUM,      C(2283))
      EQUIVALENCE   (HC,         C(2284)), (TC LN,      C(2285))
      EQUIVALENCE   (PCP(1),     C(2286)), (PCP(25),    C(2310))
      EQUIVALENCE   (DATUM(1),   C(2311)), (DATUM(3),   C(2313))
      EQUIVALENCE   (PC,         C(2314)), (TC,         C(2315))
      EQUIVALENCE   (IPROB,      C(2316)), (IFIXT,      C(2317))
      EQUIVALENCE   (IHS,        C(2318)), (ICOND,      C(2319))
      EQUIVALENCE   (ISYM,       C(2320)), (IPROD,      C(2321))
      EQUIVALENCE   (IDID,       C(2322)), (LDRUM,      C(2323))
      EQUIVALENCE   (IDRM,       C(2323)), (KDRUM,      C(2324))
      EQUIVALENCE   (L,          C(2325)), (L1,         C(2326))
      EQUIVALENCE   (M,          C(2327)), (M1,         C(2328))
      EQUIVALENCE   (N,          C(2329)), (IQ,         C(2330))
      EQUIVALENCE   (IQ1,        C(2331)), (IQ2,        C(2332))
      EQUIVALENCE   (IQ3,        C(2333)), (KMAT,       C(2334))
      EQUIVALENCE   (IMAT,       C(2335)), (IUSE,       C(2335))
      EQUIVALENCE   (IADD,       C(2336)), (ITNUMB,     C(2337))
      EQUIVALENCE   (ITAPE,      C(2338)), (P,          C(2339))
      EQUIVALENCE   (IDEBUG,     C(2340)), (IFROZ,      C(2341))
      EQUIVALENCE   (A(1),       C(2342)),  (A(1350),   C(3691))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (MCOEFT(1),  C(6392)), (MCOEFT(1350),  C(7741))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
      EQUIVALENCE (KORE, C(8047))
      EQUIVALENCE (DLNT,LNT),(SUM,MSUM),(BLK,MBLK),(TMP,MTMP),(MT,BMT)
      EQUIVALENCE    (PROD(1),  C(1538)),  (PROD(3),   C(1540))
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),      ATOM(101,3)
      DIMENSION MX(20),MCOEFT(15,90)
      DIMENSION MFORM(15)
C
B1    BMT =606060606060
B     GAS =000000000027
B     BLK =000000000060
C
      REWIND 3
      NO EQ=0
      ITEST=M1
      SIZE=18.5
  555 IF (IPROB-3) 557,563,565
  557 PC=PC/14.696006
      PO=PC
      IF (TC) 559,559,561
  559 TC LN= 8.25
      GO TO 431
  561 TC LN=LOGF(TC)
      GO TO 431
  563 PO=PC
```

```
      GO TO 431
  565 T=TC
      PO=0.0
      T LN=LOGF(T)
C
C     START CALCULATION FOR NEW OVERALL COMPOSITION
C
  431 IADD=1
      IF (IFROZ) 1565,379,1432
 1565 IF (IUSE) 1432,1432,433
 1432 DO 432 K=1,N
      EN(K)=0.0
      EN LN(K)=0.0
  432 DEL N(K)=0.0
      AAY LN=5.0
  433 SENSE LIGHT 0
      IF (IPROb-2) 435,445,434
  434 IF (IPROB-4) 455,465,379
  435 IF (IADD-1) 379,436,441
  436 SENSE LIGHT 1
  437 T LN=TC LN
      ITROT=3
  438 IF (PCP(IADD)) 231,231,439
  439 SENSE LIGHT 4
      PO=PC/PCP(IADD)
      GO TO 13
  441 IF (IADD-25) 438,438,231
  445 IF (IADD-1) 379,447,441
  447 SENSE LIGHT 2
      GO TO 437
  455 IF (IADD-25) 459,459,231
  459 IF (PCP(IADD)) 231,231,460
  460 T=PCP(IADD)
      T LN= LOGF(T)
      GO TO 473
  465 IF (IADD-25) 469,469,231
  469 IF (PCP(IADD)) 231,231,470
  470 PO=PCP(IADD)
  473 SENSE LIGHT 2
      SENSE LIGHT 4
C
C     BEGIN CALCULATIONS FOR CURRENT POINT
C
   13 PO LN=LOGF(PO)
C
C     CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
C
      IF (IPROB-2) 17,17,19
   17 T=EXPF(T LN)
   19 IF (COEFT(7,1)-T) 21,27,27
   21 IF (COEFT(7,1)-5000.0) 23,31,231
   23 DO 1123 K=1,15
      DO 1123 J = 1,90
 1123 COEFT(K,J)=COEFT1(K,J)
      SENSE LIGHT 4
      GO TO 19
   25 DO 1125 K = 1,15
      DO 1125 J = 1,90
 1125 COEFT(K,J)=COEFT2(K,J)
      SENSE LIGHT 4

      GO TO 19
   27 IF (T-COEFT(6,1)) 29,37,37
   29 IF (300.0-COEFT(6,1)) 25,31,231
   31 IF (SENSE LIGHT 4) 38,305
C
C     ELIMINATE THOSE SPECIES WHICH DO NOT HAVE DATA IN THIS INTERVAL
C
   37 IF (SENSE LIGHT 4 ) 38,142
   38 SENSE LIGHT 4
      DO 40 J=1,N
      IF (COEFT(8,J)) 40,39,4
   39 CALL BYPASS (J,2)
      EN LN(J)=0.0
      EN(J)=0.0
   40 CONTINUE
C
C     BEGIN ITERATION FOR COMPOSITION
C
   42 IQ=IQ
      IQ1=IQ1
      IQ2=IQ2
      IQ3=IQ3
      ITNUMB=30
   43 DO 48 J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 48,45,48
   45 IF (EN LN(J)+SIZE-PO LN) 46,46,47
   46 EN(J)=0.0
      GO TO 48
   47 EN(J)=EXPF(EN LN(J))
   48 CONTINUE
      IF (IPROB-2) 49,49,51
   49 T=EXPF(T LN)
   51 AAY=EXPF(AAY LN)
C
C     CALCULATE HEAT CAPACITY, ENTHALPY AND ENTROPY
C
      IFIXT=3
      IF (SENSE LIGHT 2) 52,55
   52 SENSE LIGHT 2
      IF (SENSE LIGHT 4) 53,55
   53 SENSE LIGHT 4
      IFIXT=1
      IF (ITNUMB-30) 55,54,55
   54 IFIXT=2
   55 CPSUM=0.0
      DO 60 J=1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 60,56,60
   56 IF (IFIXT-2) 59,58,57
   57 CPSUM=CPSUM+((((COEFT(12,J)*T+COEFT(11,J))*T+COEFT(10,J))*T+COEFT(
     19,J))*T+COEFT(8,J))*EN(J)
   58 HO(J)=((((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
     1+COEFT(9,J)/2.0)*T +COEFT(13,J)/T+COEFT(8,J)
   59 S(J)=((((COEFT(12,J)/4.0 )*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
     1+COEFT(9,J))*T+COEFT(8,J)*T LN+COEFT(14,J)-EN LN(J)
   60 CONTINUE
C
C     CONSTRUCT MATRIX AND SOLVE THE EQUATIONS
C
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      CALL MATRIX
      IF (SENSE LIGHT 4) 61,171
   61 SENSE LIGHT 4
      CALL GAUSS
      IF (IDEBUG) 910,80,910
  910 DO 911 I=1,IMAT
  911 WRITE OUTPUT TAPE 6,912,(G(I,K),K=1,KMAT),DELTA(I)
      WRITE OUTPUT TAPE 6,912,(X(I),I=1,IMAT)
  912 FORMAT (8E14.6)
   80 IF (IDID-IMAT) 81,85,81
   81 IF (SIZE-18.5) 83,83,311
   83 SIZE=27.5
      GO TO 43
   85 ITNUMB=ITNUMB-1
      DO 87 K=1,IMAT
      IF (ABSF(DELTA(K))-0.5E-4) 87,87,315
   87 CONTINUE
C
C     OBTAIN CORRECTIONS TO THE ESTIMATES
C
      D LN T=X(IQ2)
   91 IF (IFIXT-2) 93,95,379
   93 D LN T=0.0
   95 DO  101 J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 96,97,96
   96 DEL N(J)=0.0
      GO TO 101
   97 DEL N(J)=HO(J)*D LN T-HO(J)+S(J)
      DO  99 K=1,L
   99 DEL N(J)=DEL N(J)+A(K,J)*X(K)
  101 CONTINUE
      IF (L-IQ) 103,109,109
  103 J=M1
      DO 107 K=L1,IQ
  104 CALL BYPASS (J,1)
      IF (IPROD-2) 105,106,105
  105 DEL N(J)=0.0
      J=J+1
      GO TO 104
  106 DEL N(J)=X(K)
      J=J+1
  107 CONTINUE
  109 AMBDA=1.0
      AMBDA1=1.0
      IF (XABSF(LNT)-XABSF(MX(IQ1))) 501,913,913        — see errata
  501 SUM = ABSF(X(IQ1))
      GO TO 915
  913 SUM=ABSF(D LN T)
  915 DO 917 J=1,M
      IF (EN(J)) 917,1915,916
  916 SUM=MAX1F(DEL N(J),SUM)
      GO TO 917
 1915 IF (EN LN(J)) 917,917,1917                        — see errata
 1917 SUM1=ABSF((PO LN-9.212-EN LN(J))/DEL N(J))
      AMBDA1=MIN1F(SUM1,AMBDA1)
  917 CONTINUE
      IF (SUM-2.0) 1110,1110,110
  110 AMBDA=2.0/SUM
 1110 AMBDA=MIN1F(AMBDA,AMBDA1)

  920 IF (IDEBUG) 921,111,921
  921 WRITE OUTPUT TAPE 6,923, T,P,AAY, AMBDA, ((COEFT(K,J),K=1,3),
     1  EN(J),EN LN(J),DEL N(J),HO(J),S(J),J=1,N)
  923 FORMAT (4E25.8/(1X,3A6,5E15.6))
C
C     APPLY CORRECTIONS TO THE ESTIMATES
C
  111 DO 113 J=1,M
  113 EN LN(J)=EN LN(J)+AMBDA*DEL N(J)
      IF (ICOND-2) 115,121,375
  115 DO 117 J=M1,N
  117 EN(J)=EN(J)+AMBDA*DEL N(J)
  121 T LN=T LN +AMBDA*D LN T
      AAY LN=AAY LN- AMBDA*X(IQ1)
      IF (SENSE SWITCH 6) 122,124
  122 IF (IDEBUG) 1122,123,1122
 1122 IDEBUG=0
      GO TO 231
  123 IDEBUG=1
C
C     TEST  FOR CONVERGENCE OF ITERATION
C
  124 IF (ITNUMB) 125,132,125
  125 IF (AMBDA-1.0) 43,1124,231
 1124 P=0.0
      DO 1126 J=1,M
 1126 P=P+EXPF(EN LN(J))                                 — see errata
      IF (ABSF((PO-P)/PO)-0.5E-5) 126,126,43
  126 SUM=P
      IF(ICOND-2)127,129,375
  127 DO 128 J=M1,N
  128 SUM=SUM+ABSF(EN(J))
  129 DO 130 J=1,N
      IF (J-M) 1129,1129,1130
 1129 IF (ABSF(EN(J)*DEL N(J)/SUM)-0.5E-5) 130,130,43
 1130 IF (ABSF(DEL N(J)/SUM)-0.5E-5) 130,130,43
  130 CONTINUE
  132 IF (SENSE LIGHT 4) 133,133
  133 GO TO 13
C
C     ELIMINATE THOSE SPECIES WITH NO DATA AT THIS TEMPERATURE, ADD
C     THOSE WITH DATA AT THIS TEMPERATURE
C
  142 DO 170 J=1,N
      IF (MCOEFT(1,J)-MT) 170,500,170
  500 IF (COEFT(5,J) + 100.0-T) 285,143,143
  143 IF (T-COEFT(4,J)+100.0) 295,144,144
  285 IF (5000.0-COEFT(5,J)) 144,144,301
  295 IF (COEFT(4,J)-300.0) 144,144,301
  144 IF (J-M) 145,145,146
  145 CALL BYPASS (J,3)
      GO TO 170
  301 CALL BYPASS (J,2)
      EN(J)=0.0
      EN LN(J)=0.0
      DEL N(J)=0.0
      GO TO 170
  146 IF (EN(J)) 147,148,170
  147 EN(J)=0.0
      DEL N(J)=0.0
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      CALL BYPASS (J,2)
      GO TO 42
C
C     SKIP CONDENSATION CHECK IF T IS HIGHER THAN MELTING POINT WHEN
C     TESTING SOLID, OR LOWER THAN MELTING POINT WHEN TESTING LIQUID
C
  148 IF (COEFT(4,J)-COEFT(5,J-1)) 150,149,150
  149 IF (COEFT(4,J)-T) 153,153,170
  150 IF (COEFT(5,J)-COEFT(4,J+1)) 153,151,153
  151 IF (T-COEFT(5,J)) 153,153,170
C
C     CHECK FOR CONDENSATION
C     IF MORE THAN ONE CONDENSED PHASE OF ANY SPECIES CAN EXIST THE
C     PHASE STABLE AT THE HIGHER TEMPERATURE MUST PRECEED THAT STABLE AT
C     THE LOWER TEMPERATURE ON MASTER TAPE
C
  153 DO 155 K=2,3
      SUM=COEFT(K,J)
      DO 154 I=1,6
      TMP=ARSF(30,SUM)
B     SUM=ALSF(6000000,SUM)
      IF(MTMP-MBLK)  154,156,154
  154 CONTINUE
  155 CONTINUE
      K=3
      I=5
      GO TO 159
  156 I=I-2
      IF (I) 157,158,159
  157 K=2
      I=5
      GO TO 159
  158 K=2
      I=6
  159 FORM(2)=COEFT(2,J)
      FORM(3)=COEFT(3,J)
      I=6*I
      JJ=42-I
      I=I
      JJ=JJ
      SUM = FORM(K)
B     SUM = ARSF(JJ,SUM)
      MJJ=JJ-6
      TMLJ = FORM(K)
      TMLJ = LRSF(MJJ,TMLJ)
      MJJ=36-I
B     SUM1=LLSF(MJJ,GAS)
B     TEMP=LRSF(JJ,SUM1)
      MJJ=42-I
B     FORM(K)=LLSF(MJJ,SUM)
      DO 160 K=1,M
      IF (MFORM(2)-MCOEFT(2,K)) 160,1160,160
 1160 IF (MFORM(3)-MCOEFT(3,K)) 160,162,160
  160 CONTINUE
      CALL BYPASS (J,3)
      GO TO 170
  162 CALL BYPASS (K,1)
      IF (IPROD-2) 170,163,17
  163 HO(J)=((((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
     1+COEFT(9,J)/2.0)*T +COEFT(13,J)/T+COEFT(8,J)

      S(J)=((((COEFT(12,J)/4.0 )*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
     1+COEFT(9,J))*T+COEFT(8,J)*T LN+COEFT(14,J)
      IF (HO(J)-S(J)-HO(K)+S(K)) 164,164,170
  164 CALL BYPASS (J,3)
      EN(J)=0.0
      GO TO 42
  170 CONTINUE
C
C     IF COMPOSITION HAS BEEN CORRECTLY DETERMINED CALCULATE THE
C     EQUILIBRIUM PROPERTIES, OTHERWISE CONTINUE ITERATION
C
      IF(SENSE LIGHT 4) 1170,1172
 1170 SENSE LIGHT 4
      GO TO 42
 1172 IF (ITNUMB) 42,971,42
  971 WRITE OUTPUT TAPE 6,973,IADD
  973 FORMAT (70HL30 ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENTS
     1 FOR THE POINT I5)
      GO TO 42
C
C     CALCULATE EQUILIBRIUM PROPERTIES
C
  171 DO 1171 I = 1,454
 1171 ANS(I) = ANSLAB(I)
      WTMOL=AAY/P
      HSUM=G(IQ2,IQ1)*T/AAY
      SSUM=0.0
      DO 183 J=1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 183,181,183
  181 SSUM=SSUM+S(J)*EN(J)
  183 CONTINUE
 1183 SSUM=SSUM/AAY
      IMAT=IMAT-1
      CALL GAUSS
      IF (IDID-IMAT) 172,174,172
  172 CPR=CPSUM/AAY
      GAMMA=CPR/(CPR-(1.0/WTMOL))
      DLMTP=0.0
      DLMPT=0.0
      GO TO 185
  174 DLMTP=X(IQ1)
      IF (ABSF(DLMTP)-27.5) 1174,1174,172
 1174 CPR=G(IQ2,IQ2)
      DO 175 J=1,IQ1
  175 CPR=CPR-G(IQ2,J)*X(J)
      CPR=CPR/AAY
 1175 IMAT=IMAT-1
      CALL GAUSS
      DLMPT=0.0
      DO 179 J=1,L
  179 DLMPT=DLMPT+G(IQ1,J)*X(J)
      DLMPT=(P-DLMPT)/DLMPT
      IF (DLMPT-27.5) 180,180,172
  180 GAMMA=1.0/(1.0+DLMPT-((1.0-DLMTP)**2)/(CPR*WTMOL))
      IF (GAMMA) 172,172,185
  185 IF (IPROB-2) 186,186,207
  186 IF (IADD-2) 187,191,197
  187 WTMOLC=WTMOL
      TC=T
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      PC=P
      HC=HSUM
      SO=SSUM
  188 T PI=-DLMTP/(WTMOL*CPR)
      T ETA=1000.0/(CPR*TC*1.98726)
      T SIG=-(1.0-DLMTP)/(WTMOL*CPR)
      GO TO 207
C
C     CHECK FOR CONVERGENCE AT THROAT
C
  191 DHSTAR=HC-HSUM - (GAMMA*T/(2.0*WTMOL))
      IF (ABSF(DHSTAR/(HC-HSUM))-0.4E-4) 197,197,192
  192 IF(ITROT) 193,197,193
  193 PCP(2)=PCP(2)/(1.0+2.0*DHSTAR*WTMOL/(T*(GAMMA+1.0)))
      PO=PC/PCP(IADD)
      ITROT=ITROT-1
      IF (IDEBUG) 929,194,929
  929 WRITE OUTPUT TAPE 6,923,DHSTAR,HC,HSUM,PCP(IADD)
  194 SENSE LIGHT 4
      GO TO 13
C
C     CALCULATE PERFORMANCE PARAMETERS
C
  197 SP IMP=294.98*SQRTF((HC-HSUM)*1.98726E-3)
      RHOI=RHO*SP IMP
      SUM=T/(2.0*(HC-HSUM))
      PI I=SUM*(WTMOL-WTMOLC)/(WTMOL*WTMOLC)
      ETA I=SUM*(TC-T)/(TC*T*1.98726)*1000.0
      SIG I=SUM/WTMOL
      T PI=(((WTMOLC-WTMOL)/WTMOLC)-DLMTP)/(WTMOL*CPR)
      T ETA=1000.0/(CPR*TC*1.98726)
      T SIG=-(1.0-DLMTP)/(WTMOL*CPR)
      AW=(86.4579*T)/(AAY*14.696006*SP IMP)
      AW PI=- ((1.0-DLMTP)/(WTMOLC*CPR)+1.0/GAMMA+PI I)
      AW ETA=T ETA*(1.0-DLMTP)-ETA I
      AW SIG=1.0/GAMMA-SIG I
      IF (IADD-2) 203,201,203
  201 AWT=AW
      CSTAR=32.174*PC*14.696006*AWT
      CSTRPI=1.0+AW PI
      STR ETA=AW ETA
      STR SIG=0.0
      AWT PI=AW PI
      AWT ETA=AW ETA
      AW SIG=0.0
  203 CF=32.174*SP IMP/CSTAR
      ARATIO=AW/AWT
      VACI=SP IMP+P*14.696006*AW
      RHOVAC=RHO*VACI
      VMACH=SP IMP/SQRTF(86.4579*GAMMA*T/WTMOL)
      EP PI=AW PI-AWT PI
      EP ETA=AW ETA-AWT ETA
      EP SIG=AW SIG
  207 HSUM=HSUM*1.98726
      SSUM=SSUM*1.98726
      CP=CPR*1.98726
C
C     OBTAIN COMPOSITION IN MOLE FRACTIONS
C
      SUM=P


      IF (ICOND-2) 209,213,375
  209 DO 211 J=M1,N
  211 SUM=SUM+EN(J)
  213 DO 215 J=1,N
  215 ANS(4*J+34)=EN(J)/SUM
      IF (IPROB-2) 217,217,22
  217 ANS(1)=PCP(IADD)
  218 IF (IADD-2) 220,219,219
  219 ANS(15)=CSTAR
      ANS(24)=CSTRPI
      ANS(29)=STR ETA
      ANS(34)=STR SIG
  220 ANS(2)=P
      ANS(3)=T
      K=34+4*N
C
C     PRINT OUT THE CALCULATED ANSWERS
C
      IF (IDEBUG) 1221,222,1221
 1221 WRITE OUTPUT TAPE 6,221,(ANS(I),I=1,K)
  221 FORMAT (1H ////5E20.8/5E20.8/5E20.8/4E20.8/5E20.8/5E20.8/5E20.8///
     1 (3(7X,3A6,F8.5)))
      GO TO 2223
  222 WRITE TAPE 3, (ANS(I), I=1,454)
      NO EQ=NO EQ+1
 2223 IF (IADD-2) 223,225,225
  223 IF (IPROB-2) 224,1224,1223
  224 IF (IFROZ) 1223,1224,1224
 1224 PCP(2)=((GAMMA+1.0)/2.0)**(GAMMA/(GAMMA-1.0))
      T LN=T LN+LOGF(2.0/(GAMMA+1.0))
 1223 DO 1225 I = 1,454
 1225 ANSLAB(I) = ANS(I)
  225 IADD=IADD+1
      GO TO 433
C
  231 IF (NO EQ) 378,378,1231
 1231 IF (IFROZ) 232,379,235
  232 IF (IADD-2) 378,233,378
  233 IF (IDEBUG) 378,234,378
  234 CALL  CORE4
      IF (KORE) 1234,1,1234
 1234 RETURN
  235 IF (IPROB-2) 237,237,239
  237  CALL CORE3
      RETURN
  239 WRITE TAPE 3,(G(I), I=1,8044)
      CALL CORE5
      RETURN
C
C     ERROR PRINT OUT
C
  305 WRITE OUTPUT TAPE 6,306,T,IADD
  306 FORMAT (17HLTHE TEMPERATURE=E12.4,34H K, IS OUT OF RANGE FOR THE P
     1OINT I5)
      IF (6000.0-T) 309,307,307
  307 IF (T-200.0) 1309,308,308
  308 GO TO 142
 1309 IF (IADD-1) 309,1310,309
 1310 IF (IPROB-2) 1311,309,309
 1311 IF (ITEST-N) 1312,1312,309
```

```
1312 DO 1313 J=ITEST,N
     CALL BYPASS(J,1)
     IF (IPROD-2) 1315,1313,1313
1313 CONTINUE
     GO TO 309
1315 ITEST=J+1
     CALL BYPASS(J,3)
     GO TO 555
 309 IADD=25
     IF (SENSE LIGHT 4) 42,42
 311 WRITE OUTPUT TAPE 6,312,IMAT,IDID
 312 FORMAT (/15H1TRIED TO SOLVE I3,22H EQUATIONS, ELIMINATED I3)
     GO TO 375
 315 WRITE OUTPUT TAPE 6,316,
 316 FORMAT (/47H1RESIDUALS FROM SUBROUTINE GAUSS EXCEED  0.5E-4)
 375 IF (IDEBUG) 231,377,231
 377 IDEBUG=1
     IF (IPROB-3) 1377,555,555
1377 PC=PC*14.696006
     GO TO 555
 378 WRITE TAPE 3,(G(I),I=1,8044)
     BACKSPACE 3
     RETURN
```

see errata

```
  379 REWIND 4
      PAUSE 77777
      SUBROUTINE  GAUSS
C
C
C     SUBROUTINE GAUSS SOLVES ANY LINEAR SET OF UP TO TWENTY EQUATIONS,
C     BY ITERATION IF NECESSARY
C
C     FORTRAN MONITOR UNDER NORMAL OPERATING CONDITIONS WILL TAKE CARE
C     OF OVER-UNDER FLOW
C
      COMMON C
      EQUIVALENCE   (G(1),      C(1)),     (G(420),     C(420))
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),    C(874))
      EQUIVALENCE   (HSUM,      C(424)),   (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,     C(426)),   (CP,         C(427))
      EQUIVALENCE   (DLMPT,     C(428)),   (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,     C(430)),   (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,     C(432)),   (SP IMP,     C(433))
      EQUIVALENCE   (VACI,      C(434)),   (CF,         C(436))
      EQUIVALENCE   (RHOI,      C(437)),   (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,       C(439))
      EQUIVALENCE   (T PI,      C(440)),   (PI I,       C(441))
      EQUIVALENCE   (EP PI,     C(442)),   (AW PI,      C(443))
      EQUIVALENCE   (T ETA,     C(445))
      EQUIVALENCE   (ETA I,     C(446)),   (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,    C(448)),   (T SIG,      C(450))
      EQUIVALENCE   (SIG I,     C(451)),   (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,    C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),   C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (ELMT(1),   C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE   (LLMT(1),   C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE   (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,     C(1472)),  (JEAN,     C(1473))
      EQUIVALENCE   (ACX,      C(1474)),  (ACF,     C(1475))
      EQUIVALENCE   (AMX,       C(1476)),  (AMF,      C(1477))
      EQUIVALENCE   (RHOX,      C(1478)),  (RHOF,    C(1479))
      EQUIVALENCE   (COEFX(1),    C(1480)),  (COEFX(20), C(1499))
      EQUIVALENCE   (DX(1),    C(1500)),  (DX(20),   C(1519))
      EQUIVALENCE   (FORMLA(1), C(1520)),  (FORMLA(18), C(1537))
      EQUIVALENCE   (MMLA(1),   C(1520)),  (MMLA(18), C(1537))
      EQ'JIVALENCE   (PROD(1),  C(1538)),  (PROD(3),   C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),  (SYSTM(15),  C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,      C(1556)),      (FPCT,   C(1557))
      EQUIVALENCE   (EQRAT,     C(1558))
      EQUIVALENCE (KODE,    C(1559)),   (KASE,       C(1560))
      EQUIVALENCE   (KONT,   C(1561)),    (NF,          C(1562))
      EQUIVALENCE   (NO,        C(1563)), (NE,          C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (BOX(1),    C(1771)), (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),    C(1786)), (BOF(15),   C(1800))
      EQUIVALENCE   (HX,        C(1801)), (HF,        C(1802))
      EQUIVALENCE   (VXPLS,     C(1803)), (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,     C(1805)), (VFMIN,     C(1806))
      EQUIVALENCE   (EN LN(1),  C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),  C(1951)), (DEL N(90), C(2040))

      EQUIVALENCE   (HO(1),     C(2041)), (HO(90),    C(2130))
      EQUIVALENCE   (S(1),      C(2131)), (S(90),     C(2220))
      EQUIVALENCE   (X(1),      C(2221)), (X(20),     C(2240))
      EQUIVALENCE   (DELTA(1),  C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (BO(1),     C(2261)), (BO(15),    C(2275))
      EQUIVALENCE   (PO,        C(2276)), (HSUBO,     C(2277))
      EQUIVALENCE   (SO,        C(2278)), (T LN,      C(2279))
      EQUIVALENCE   (T,         C(2280)), (AAY LN,    C(2281))
      EQUIVALENCE   (AAY,       C(2282)), (CPSUM,     C(2283))
      EQUIVALENCE   (HC,        C(2284)), (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),    C(2286)), (PCP(25),   C(2310))
      EQUIVALENCE   (DATUM(1),  C(2311)), (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,        C(2314)), (TC,        C(2315))
      EQUIVALENCE   (IPROB,     C(2316)), (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,       C(2318)), (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,      C(2320)), (IPROD,     C(2321))
      EQUIVALENCE   (IDID,      C(2322)), (LDRUM,     C(2323))
      EQ'JIVALENCE   (IDRM,      C(2323)), (KDRUM,     C(2324))
      EQUIVALENCE   (L,         C(2325)), (L1,        C(2326))
      EQUIVALENCE   (M,         C(2327)), (M1,        C(2328))
      EQUIVALENCE   (N,         C(2329)), (IQ,        C(2330))
      EQUIVALENCE   (IQ1,       C(2331)), (IQ2,       C(2332))
      EQUIVALENCE   (IQ3,       C(2333)), (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,      C(2335)), (IUSE,      C(2335))
      EQUIVALENCE   (IADD,      C(2336)), (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,     C(2338)), (P,         C(2339))
      EQUIVALENCE   (IDEBUG,    C(2340)), (IFROZ,     C(2341))
      EQUIVALENCE   (A(1),      C(2342)),  (A(1350),  C(3691))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
C
      DIMENSION   G(20,21),   A(15,90),     EN(90),       EN LN(90)
      DIMENSION   DEL N(90),  HO(90),       S(90),        X(20)
      DIMENSION   DELTA(20),  BO(15),       PCP(25),      PROD(3)
      DIMENSION   COEFX(20),  DX(20),       FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),     DATUM(3),     FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),      ANS(454),     SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),    COEFT(15,90)
      DIMENSION   MATOM(101,3),      ATOM(101,3)
      DIMENSION  DRUM(20,21)
8     BIGNO=377777777777
      IDID=0
      DETN=0.0
      IF(IUSE) 80,80,81
   81 IUSE1=IUSE+1
      DO 1 K=1,IUSE
      X(K)=0.0
    1 DELTA(K)=0.0
      ITERA=0
      KAPUT=1
      DSUM1=BIGNO
C
C     SAVE MATRIX IN DRUM
C
      DO 82 ID=1,IUSE
```

```
      DO82  JN=1, IUSE1
   82 DRUM(ID,JN)=G(ID,JN)
C
C     BEGIN ELIMINATION OF NNTH VARIABLE
C
    6 DO 45 NN=1,IUSE
      IF (NN-IUSE) 8,83,8
   83 IF(G(NN,NN))31,23,31
C
C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW
C
    8 DO 18 I=NN,IUSE
      J=NN
      IF(G(I,J)) 99,14,99
   99 COEFX(I)=0.0
   10 J=J+1
      IF(IUSE1-J) 12,84,84
   84 IF( ABSF(G(I,J)) - ABSF(COEFX(I))) 10,100,100
  100 COEFX(I)=ABSF(G(I,J))
      GO TO 10
   12 COEFX(I)= ABSF(COEFX(I)/G(I,NN))
      GO TO 18
   14 COEFX(I)=BIGNO
   18 CONTINUE
   19 TEMP=BIGNO
      I=0
   20 DO 22 J=NN,IUSE
      IF (COEFX(J)-TEMP) 87,22,22
   87 TEMP=COEFX(J)
      I=J
   22 CONTINUE
      IF(I) 28,23,28
   23 IDID=NN-1
      GO TO 80
C
C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
C     VARIABLE FROM THE REMAINING EQUATIONS
C
C      INTERCHANGE EQUATIONS I AND NN
C
   28 IF(NN-I) 29,31,29
   29 DO 30 J=NN,IUSE1
      Z=G(I,J)
      G(I,J)=G(NN,J)
   30 G(NN,J)=Z
C
C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
C     VARIABLE FROM THE REMAINING EQUATIONS
C
   31 K = NN + 1
      DO 36 J = K, IUSE1
            IF(G(NN,NN)) 36, 23, 36
   36       G(NN,J) = G(NN,J) / G(NN,NN)
      IF(K-IUSE1) 88,45,88
   88 DO 44 I = K,IUSE
   40 DO 44 J = K, IUSE1
            G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
   44 CONTINUE
   45 CONTINUE
C

C     BACKSOLVE FOR THE VARIABLES
C
  991 IDID = IUSE
      K = IUSE
   47 J = K + 1
      SUM = 0.
      IF(IUSE - J) 51,48,48
   48 DO 50 I = J,IUSE
   50       SUM = SUM + G(K,I)*DX(I)
   51 DX(K) = G(K,IUSE1) - SUM
      X(K) = X(K) + DX(K)
      K = K - 1
      IF (K) 47,151,47
  151 DO 90 ID = 1,IUSE
      DO 90 JD = 1, IUSE1
   90       G(ID,JD) = DRUM(ID,JD)
C
C     CALCULATE RESIDUALS (DELTA RIGHT HAND SIDE)
C
   52 DSUM = 0.
      DO 62 I = 1, IUSE
            SUM = 0.
            DO 56 J = 1, IUSE
   56             SUM = SUM + G(I,J)*X(J)
            DELTA(I) = G(I,IUSE1) - SUM
            IF(ABSF(G(I,IUSE1)) - 1.0) 62, 62, 6
   60       DELTA(I) = DELTA(I) / G(I,IUSE1)
   62       DSUM = ABSF(DELTA(I)) + DSUM
      GO TO(66,80), KAPUT
   66 IF(DSUM - DSUM1) 74,80,68
   68 KAPUT = 2
      DO 72 K = 1,IUSE
   72       X(K) = X(K) - DX(K)
      GO TO 52
   74 DSUM1 = DSUM
      ITERA = ITERA + 1
      IF(ITERA -  4) 92,80,92
   92 DO 78 I = 1,IUSE
            IF(ABSF(G(I,IUSE1)) - 1.0) 75,75,76
   75       G(I,IUSE1) = DELTA(I)
            GO TO 78
   76       G(I,IUSE1) = DELTA(I) * G(I,IUSE1)
   78       CONTINUE
      GO TO 6
   80 RETURN
```

```
      SUBROUTINE MATRIX
C
C
      COMMON C
      EQUIVALENCE   (G(1),      C(1)),    (G(420),     C(420))
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),     C(874))
      EQUIVALENCE   (HSUM,      C(424)),  (SSUM,       C(425))
      EQUIVALENCE   (WTMOL,     C(426)),  (CP,         C(427))
      EQUIVALENCE   (DLMPT,     C(428)),  (DLMTP,      C(429))
      EQUIVALENCE   (GAMMA,     C(430)),  (ARATIO,     C(431))
      EQUIVALENCE   (VMACH,     C(432)),  (SP IMP,     C(433))
      EQUIVALENCE   (VACI,      C(434)),  (CF,         C(436))
      EQUIVALENCE   (RHOI,      C(437)),  (RHOVAC,     C(438))
      EQUIVALENCE   (RHO,       C(439))
      EQUIVALENCE   (T PI,      C(440)),  (PI I,       C(441))
      EQUIVALENCE   (EP PI,     C(442)),  (AW PI,      C(443))
      EQUIVALENCE   (T ETA,     C(445))
      EQUIVALENCE   (ETA I,     C(446)),  (EP ETA,     C(447))
      EQUIVALENCE   (AW ETA,    C(448)),  (T SIG,      C(450))
      EQUIVALENCE   (SIG I,     C(451)),  (EP SIG,     C(452))
      EQUIVALENCE   (AW SIG,    C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),   C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (ELMT(1),   C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE   (LLMT(1),   C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE   (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,     C(1472)),   (JEAN,     C(1473))
      EQUIVALENCE   (ACX,      C(1474)),   (ACF,     C(1475))
      EQUIVALENCE   (AMX,       C(1476)),   (AMF,      C(1477))
      EQUIVALENCE   (RHOX,      C(1478)),   (RHOF,    C(1479))
      EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),     C(1500)),  (DX(20),    C(1519))
      EQUIVALENCE   (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),   C(1520)),  (MMLA(18), C(1537))
      EQUIVALENCE   (PROD(1),  C(1538)),  (PROD(3),    C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),  (SYSTM(15),   C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,      C(1556)),     (FPCT,   C(1557))
      EQUIVALENCE   (EQRAT,     C(1558))
      EQUIVALENCE (KODE,     C(1559)),   (KASE,      C(1560))
      EQUIVALENCE   (KONT,   C(1561)),    (NF,        C(1562))
      EQUIVALENCE   (NO,        C(1563)), (NE,        C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (BOX(1),    C(1771)), (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),    C(1786)), (BOF(15),   C(1800))
      EQUIVALENCE   (HX,        C(1801)), (HF,        C(1802))
      EQUIVALENCE   (VXPLS,     C(1803)), (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,     C(1805)), (VFMIN,     C(1806))
      EQUIVALENCE   (EN LN(1),  C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),  C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (HO(1),     C(2041)), (HO(90),    C(2130))
      EQUIVALENCE   (S(1),      C(2131)), (S(90),     C(2220))
      EQUIVALENCE   (X(1),      C(2221)), (X(20),     C(2240))
      EQUIVALENCE   (DELTA(1),  C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (BO(1),     C(2261)), (BO(15),    C(2275))
      EQUIVALENCE   (PO,        C(2276)), (HSUBO,     C(2277))
      EQUIVALENCE   (SO,        C(2278)), (T LN,      C(2279))
      EQUIVALENCE   (T,         C(2280)), (AAY LN,    C(2281))

      EQUIVALENCE   (AAY,       C(2282)), (CPSUM,     C(2283))
      EQUIVALENCE   (HC,        C(2284)), (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),    C(2286)), (PCP(25),   C(2310))
      EQUIVALENCE   (DATUM(1),  C(2311)), (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,        C(2314)), (TC,        C(2315))
      EQUIVALENCE   (IPROB,     C(2316)), (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,       C(2318)), (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,      C(2320)), (IPROD,     C(2321))
      EQUIVALENCE   (IDID,      C(2322)), (LDRUM,     C(2323))
      EQUIVALENCE   (IDRM,      C(2323)), (KDRUM,     C(2324))
      EQUIVALENCE   (L,         C(2325)), (L1,        C(2326))
      EQUIVALENCE   (M,         C(2327)), (M1,        C(2328))
      EQUIVALENCE   (N,         C(2329)), (IQ,        C(2330))
      EQUIVALENCE   (IQ1,       C(2331)), (IQ2,       C(2332))
      EQUIVALENCE   (IQ3,       C(2333)), (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,      C(2335)), (IUSE,      C(2335))
      EQUIVALENCE   (IADD,      C(2336)), (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,     C(2338)), (P,         C(2339))
      EQUIVALENCE   (IDEBUG,    C(2340)), (IFROZ,     C(2341))
      EQUIVALENCE   (A(1),      C(2342)),  (A(1350),  C(3691))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),     ATOM(101,3)
C
C
C     DETERMINE WHICH MATRIX IS TO BE SET UP
C     SENSE LIGHT        LIGHT ON                  LIGHT OFF
C          1          COMBUSTION TYPE           EXPANSION TYPE
C          2          ASSIGNED TEMPERATURE      UNASSIGNED TEMPERATURE
C          4          NOT CONVERGED             CONVERGED
C
      IQ1=IQ1
      IQ2=IQ2
      IQ3=IQ3
      IF (SENSE LIGHT 2) 1,4
    1 SENSE LIGHT 2
      IF (SENSE LIGHT 4) 2,3
    2 SENSE LIGHT 4
      IFIXT=1
      ISYM=IQ1
      GO TO 10
    3 IFIXT=2
      IHS=1
      ISYM=IQ2
      GO TO 10
    4 IFIXT=2
      IF (SENSE LIGHT 1) 5,6
```

```
    5 SENSE LIGHT 1
      IHS=1
      ISYM= IQ2
      GO TO 10
    6 IF (SENSE LIGHT 4) 7, 8
    7 SENSE LIGHT 4
      IHS=2
      ISYM=IQ1
      GO TO 10
    8 IHS=1
      ISYM=IQ2
C
C     CLEAR MATRIX STORAGES TO ZERO
C
   10 DO 212 I=1,IQ2
      DO 211 K=1,IQ3
      G(I,K)= 0.0
  211 CONTINUE
  212 CONTINUE
      ICOND=1
      IF (L-IQ) 14,213,14
  213 ICOND=2
C
C     BEGIN SET UP OF ITERATION MATRIX
C
   14 DO 65  J=1,M
      CALL BYPASS (J,1)
      IF (IPROD-2) 65,214,65
  214 IF (EN(J)) 65,65,12
C
C     CALCULATE THE ELEMENTS  R(I,K)
C
   12 DO 20  I=1, L
      IF (A(I,J)) 13,20,13
   13 TERM= A(I,J)*EN(J)
      DO 15  K=I, L
      G(I,K)= G(I,K) + A(K,J)*TERM
   15 CONTINUE
C
C     COMPLETE COLUMN  A FOR THE GAS MOLECULE
C
      G(I,IQ1)=G(I,IQ1)+TERM
   20 CONTINUE
      G(IQ1,IQ1)= G(IQ1,IQ1)+EN(J)
C
C     STATEMENT 24 IS FOR FIXED T, 30 IS FOR VARIABLE  T AND CONVERGED
C     FIXED T
C
   21 IF (IFIXT-2) 24,30,30
C
C     FOR ASSIGNED T BYPASS ENERGY ROW AND T COLUMN WHILE ITERATING
C
   24 TERM= (HO(J)-S(J))*EN(J)
      DO 25  I=1, L
      G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM
   25 CONTINUE
      G(IQ1,IQ2)=G(IQ1,IQ2)+TERM
      GO TO 65
C
C     FILL IN TEMPERATURE COLUMN AND RIGHT HAND SIDE

C
   30 TERM=HO(J)*EN(J)
      DO 35 I=1,L
      G(I,IQ2)= G(I,IQ2)+A(I,J)*TERM
   35 CONTINUE
      G(IQ1,IQ2)= G(IQ1,IQ2)+TERM
      TERM1=(HO(J)-S(J))*EN(J)
      DO 40 I=1,L
      G(I,IQ3)= G(I,IQ3)+A(I,J)*TERM1
   40 CONTINUE
      G(IQ1,IQ3)=G(IQ1,IQ3)+TERM1
C
C     STATEMENT 50 IS FOR ENTHALPY , 55 IS FOR ENTROPY EQUATION
C
   45 IF (IHS-2) 50,55,55
   50 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM
      G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*TERM1
      GO TO 65
C
C     DURING EXPANSION THE ENTROPY ROW IS FILLED IN
C
   55 TERM=S(J)*EN(J)
      DO 60  K=1,L
   60 G(IQ2,K)= G(IQ2,K)+A(K,J)*TERM
      CONTINUE
      G(IQ2,IQ1)=G(IQ2,IQ1)+TERM
      G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*TERM
      G(IQ2,IQ3)=G(IQ2,IQ3)+(HO(J)-S(J))*TERM
   65 CONTINUE
C
C     AT THIS POINT PROCESSING OF GASEOUS PRODUCTS HAS BEEN COMPLETED
C     AND CONDENSED PHASE PROCESSING IS BEGUN
C
C     STATEMENT 70 IS FOR CONDENSED PRODUCTS, 101 IS FOR NO CONDENSED
C
   66 IF (ICOND-2) 70,101,101
   70 K=L1
      DO 100 J= M1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 100,74,100
   74 DO 75  I=1,L
      G(I,K)=A(I,J)
   75 CONTINUE
C
C     STATEMENT 80 IS FOR FIXED T, 85 IS FOR VARIABLE T AND CONVERGED
C     FIXED T
C
      IF (IFIXT-2) 80,85,85
   80 G(K,IQ2)= HO(J)-S(J)
      GO TO 95
   85 G(K,IQ2)= HO(J)
      G(K,IQ3)= HO(J)-S(J)
C
C     STATEMENT 95 IS FOR ENTHALPY, STATEMENT 90 IS FOR ENTROPY EQUATION
C
      IF (IHS-2) 95,90,90
   90 G(IQ2,K)=S(J)
   95 K= K+1
  100 CONTINUE
C
```

```
C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX BEFORE COMPLETING THE
C     CONDENSED PHASE CONTRIBUTIONS TO THE MATRIX
C
  101 DO 104 I=1,ISYM
      DO 102 J=I,ISYM
      G(J,I)=G(I,J)
  102 CONTINUE
  104 CONTINUE
C
C     THE ADDRESS OF THE NEXT INSTRUCTION IF SET DURING INITIALIZATION
C     STATEMENT 105 IS FOR CONDENSED,130  IS FOR NO CONDENSED
C
      IF (ICOND-2) 105,130,13
C
C     COMPLETE COLUMN A OF MATRIX
C
  105 DO 125 J=M1,N
      CALL BYPASS (J,1)
      IF (IPROD-2) 125,106,125
  106 DO 107 I=1,L
      G(I,IQ1)=G(I,IQ1)+A(I,J)*EN(J)
  107 CONTINUE
      IF (IFIXT-2) 125,109,109
  109 IF (IHS-2) 110,115,115
  110 G(IQ2,IQ1)= G(IQ2,IQ1)+HO(J)*EN(J)
      GO TO 125
  115 G(IQ2,IQ1)= G(IQ2,IQ1)+S(J)*EN(J)
  125 CONTINUE
  130 GO TO (131,133),IFIXT
  131 KMAT=IQ2
      GO TO 136
  133 KMAT=IQ3
  136 IMAT=KMAT-1
C
C     COMPLETE THE RIGHT HAND SIDE
C
      DO 145 I=1,IMAT
      G(I,KMAT)=G(I,KMAT)-G(I,IQ1)
  145 CONTINUE
      DO 150 I=1,L
      G(I,KMAT)= G(I,KMAT)+ AAY*80(I)
  150 CONTINUE
      P= G(IQ1,IQ1)
  160 G(IQ1,KMAT) = G(IQ1,KMAT)+ PO
      G(IQ1,IQ1)=0.0
C
C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
C
      IF (KMAT-IQ2) 165,185,165
  165 IF (IHS-2) 166,168,168
  166 ENERGY=AAY*(HSUBO/T)
      GO TO 169
  168 ENERGY= AAY*S0+PO-P
  169 G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY
      G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM
  185 RETURN
```

```
      SUBROUTINE  CORE3
C
C     FROZEN COMPOSITION EXPANSION
C
C
      COMMON C
      EQUIVALENCE  (G(1),      C(1)),    (G(420),     C(420))
      EQUIVALENCE  (ANS(1),  C(421)),  (ANS(454),     C(874))
      EQUIVALENCE  (HSUM,      C(424)),  (SSUM,       C(425))
      EQUIVALENCE  (WTMOL,     C(426)),  (CP,         C(427))
      EQUIVALENCE  (DLMPT,     C(428)),  (DLMTP,      C(429))
      EQUIVALENCE  (GAMMA,     C(430)),  (ARATIO,     C(431))
      EQUIVALENCE  (VMACH,     C(432)),  (SP IMP,     C(433))
      EQUIVALENCE  (VACI,      C(434)),  (CF,         C(436))
      EQUIVALENCE  (RHOI,      C(437)),  (RHOVAC,     C(438))
      EQUIVALENCE  (RHO,       C(439))
      EQUIVALENCE  (T PI,      C(440)),  (PI I,       C(441))
      EQUIVALENCE  (EP PI,     C(442)),  (AW PI,      C(443))
      EQUIVALENCE  (T ETA,     C(445))
      EQUIVALENCE  (ETA I,     C(446)),  (EP ETA,     C(447))
      EQUIVALENCE  (AW ETA,    C(448)),  (T SIG,      C(450))
      EQUIVALENCE  (SIG I,     C(451)),  (EP SIG,     C(452))
      EQUIVALENCE  (AW SIG,    C(453))
      EQUIVALENCE  (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE  (FORM(1),   C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE  (ELMT(1),   C(1344)),  (ELMT(15), C(1358))
      EQUIVALENCE  (LLMT(1),   C(1344)),  (LLMT(15), C(1358))
      EQUIVALENCE  (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE  (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE  (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE  (ISYS,     C(1472)),   (JEAN,    C(1473))
      EQUIVALENCE  (ACX,      C(1474)),   (ACF,    C(1475))
      EQUIVALENCE  (AMX,       C(1476)),   (AMF,      C(1477))
      EQUIVALENCE  (RHOX,      C(1478)),   (RHOF,    C(1479))
      EQUIVALENCE  (COEFX(1),    C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE  (DX(1),    C(1500)),  (DX(20),    C(1519))
      EQUIVALENCE  (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
      EQUIVALENCE  (MMLA(1),   C(1520)),  (MMLA(18), C(1537))
      EQUIVALENCE  (PROD(1),  C(1538)),  (PROD(3),   C(1540))
      EQUIVALENCE  (SYSTM(1),  C(1541)),  (SYSTM(15),   C(1555))
      EQUIVALENCE  (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE  (OF,      C(1556)),      (FPCT,   C(1557))
      EQUIVALENCE  (EQRAT,     C(1558))
      EQUIVALENCE (KODE,     C(1559)),    (KASE,       C(1560))
      EQUIVALENCE  (KONT,   C(1561)),    (NF,          C(1562))
      EQUIVALENCE  (NO,         C(1563)), (NE,         C(1564))
      EQUIVALENCE  (NOEQ, C(1565))
      EQUIVALENCE (NOFROZ,  C(1566))
      EQUIVALENCE  (BOX(1),     C(1771)), (BOX(15),    C(1785))
      EQUIVALENCE  (BOF(1),     C(1786)), (BOF(15),    C(1800))
      EQUIVALENCE  (HX,         C(1801)), (HF,         C(1802))
      EQUIVALENCE  (VXPLS,      C(1803)), (VXMIN,      C(1804))
      EQUIVALENCE  (VFPLS,      C(1805)), (VFMIN,      C(1806))
      EQUIVALENCE  (EN LN(1),   C(1861)), (EN LN(90),  C(1950))
      EQUIVALENCE  (DEL N(1),   C(1951)), (DEL N(90),  C(2040))
      EQUIVALENCE  (HO(1),      C(2041)), (HO(90),     C(2130))
      EQUIVALENCE  (S(1),       C(2131)), (S(90),      C(2220))
      EQUIVALENCE  (X(1),       C(2221)), (X(20),      C(2240))
      EQUIVALENCE  (DELTA(1),   C(2241)), (DELTA(20),  C(2260))
      EQUIVALENCE  (BO(1),      C(2261)), (BO(15),     C(2275))

      EQUIVALENCE  (PO,         C(2276)), (HSUBO,      C(2277))
      EQUIVALENCE  (SO,         C(2278)), (T LN,       C(2279))
      EQUIVALENCE  (T,          C(2280)), (AAY LN,     C(2281))
      EQUIVALENCE  (AAY,        C(2282)), (CPSUM,      C(2283))
      EQUIVALENCE  (HC,         C(2284)), (TC LN,      C(2285))
      EQUIVALENCE  (PCP(1),     C(2286)), (PCP(25),    C(2310))
      EQUIVALENCE  (DATUM(1),   C(2311)), (DATUM(3),   C(2313))
      EQUIVALENCE  (PC,         C(2314)), (TC,         C(2315))
      EQUIVALENCE  (IPROB,      C(2316)), (IFIXT,      C(2317))
      EQUIVALENCE  (IHS,        C(2318)), (ICOND,      C(2319))
      EQUIVALENCE  (ISYM,       C(2320)), (IPROD,      C(2321))
      EQUIVALENCE  (IDID,       C(2322)), (LDRUM,      C(2323))
      EQUIVALENCE  (IDRM,       C(2323)), (KDRUM,      C(2324))
      EQUIVALENCE  (L,          C(2325)), (L1,         C(2326))
      EQUIVALENCE  (M,          C(2327)), (M1,         C(2328))
      EQUIVALENCE  (N,          C(2329)), (IQ,         C(2330))
      EQUIVALENCE  (IQ1,        C(2331)), (IQ2,        C(2332))
      EQUIVALENCE  (IQ3,        C(2333)), (KMAT,       C(2334))
      EQUIVALENCE  (IMAT,       C(2335)), (IUSE,       C(2335))
      EQUIVALENCE  (IADD,       C(2336)), (ITNUMB,     C(2337))
      EQUIVALENCE  (ITAPE,      C(2338)), (P,          C(2339))
      EQUIVALENCE  (IDEBUG,     C(2340)), (IFROZ,      C(2341))
      EQUIVALENCE  (A(1),       C(2342)),  (A(1350),  C(3691))
      EQUIVALENCE  (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE  (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE  (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE  (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE  (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
C
      DIMENSION   G(20,21),   A(15,90),   EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),     S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),     PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),     FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),   DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),    ANS(454),   SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),     ATOM(101,3)
C
C
      NO FROZ=0
      MISSED=0
      DO 1004 J = 1,454
 1004 ANS(J) = ANSLAB(J)
    4 IADD=1
      ITROT=3
      ALPHA=0.0
      DO 7 J=1,N
      EN(J)=ANS(4*J+34)
      IF (EN(J)) 6,6,15
   15 IF (J-M) 5,5,7
    5 EN LN(J)=LOGF(EN(J))
      ALPHA=ALPHA+EN(J)
      GO TO 7
    6 EN LN(J)=0.0
      EN(J)=0.0
    7 CONTINUE
      WTMOLF=ALPHA*WTMOL
      PC=ANS(2)
```

```
      T LN=LOGF(ANS(3))
      HC=ANS(4)/1.98726
      SO= (ANS(5)*WTMOLF/1.98726)+ALPHA*LOGF(PC/ALPHA)
      DLMPT=0.0
      DLMTP=0.0
C
C     BEGIN CALCULATIONS FOR CURRENT POINT
C     CHECK TEMPERATURE RANGE OF THERMODYNAMIC DATA
C
      DO 1117 J=1,454
 1117 ANSLAB(J)=ANS(J)
   17 T=EXPF(T LN)
   19 IF (COEFT(7,1)-T) 21,27,27
   21 IF (COEFT(7,1)-5000.0) 23,22,451
   22 IF (IADD-2) 51,31,31
   23 DO 1123 K = 1,15
      DO 1123 J = 1,90
 1123 COEFT(K,J) = COEFT1(K,J)
      SENSE LIGHT 4
      GO TO 19
   25 DO 1125 K = 1,15
      DO 1125 J = 1,90
 1125 COEFT(K,J)=COEFT2(K,J)
      SENSE LIGHT 4
      GO TO 19
   27 IF (T-COEFT(6,1)) 29,35,35
   29 IF (300.0-COEFT(6,1)) 25,22,451
   31 IF (SENSE LIGHT 4) 38,305
C
C     LEAVE FROZEN PROGRAM IF DATA FOR ANY SPECIES RUNS OUT
C
   35 IF (IADD-2) 51,37,37
   37 IF (SENSE LIGHT 4) 38,41
   38 SENSE LIGHT 4
      DO 40 J=1,N
      IF (COEFT(8,J)) 40,39,4
   39 IF (EN(J)) 40,40,309
   40 CONTINUE
      GO TO 49
   41 DO 44 J=1,N
      IF (EN(J)) 44,44,42
   42 IF (COEFT(5,J)+20.0-T) 285,43,43
   43 IF (T-COEFT(4,J)+20.0) 295,44,44
  285 IF (5000.0-COEFT(5,J)) 44,44,311
  295 IF (COEFT(4,J)-300.0) 44,44,311
   44 CONTINUE
C
C     BEGIN ITERATION
C
   49 PCP LN=LOGF(PCP(IADD))
   51 CPSUM=0.0
      T=EXPF(T LN)
      DO 60 J=1,N
      IF (EN(J)) 60,60,57
   57 CPSUM=CPSUM+((((COEFT(12,J)*T+COEFT(11,J))*T+COEFT(10,J))*T+COEFT(
     19,J))*T+COEFT(8,J))*EN(J)
   58 HO(J)=((((COEFT(12,J)/5.0)*T+COEFT(11,J)/4.0)*T+COEFT(10,J)/3.0)*T
     1+COEFT(9,J)/2.0)*T +COEFT(13,J)/T+COEFT(8,J)
   59 S(J)=((((COEFT(12,J)/4.0 )*T+COEFT(11,J)/3.0)*T+COEFT(10,J)/2.0)*T
     1 +COEFT(9,J))*T+COEFT(8,J)*T LN+COEFT(14,J)-EN LN(J)

   60 CONTINUE
      SUM H=0.0
      SUM S=0.0
      DO 63 J=1,N
      SUM H=SUM H+HO(J)*EN(J)
   63 SUM S=SUM S+S(J)*EN(J)
      IF (IADD-2) 81,65,65
   65 IF (SENSE LIGHT 4) 66,81
   66 SENSE LIGHT 4
   67 D LN T=(SUM S+(ALPHA*PCP LN)-SO)/CPSUM
C
C     CHECK CONVERGENCE OF THE ITERATION
C
      T LN=T LN-D LN T
      IF (ABSF(D LN T)-0.5E-4) 73,73,51
   73 IF (SENSE LIGHT 4) 17,17
   81 DO 1181 J = 1,454
 1181 ANS(J) = ANSLAB(J)
      SUM H=T*SUM H/WTMOLF
      CPR=CPSUM/WTMOLF
      GAMMA=CPR/(CPR-(1.0/WTMOL))
      IF (IADD-2) 209,191,197
C
C     CHECK FOR CONVERGENCE AT THROAT
C
  191 DHSTAR=HC-SUM H - (GAMMA*T/(2.0*WTMOL))
      IF (ABSF(DHSTAR/(HC-SUM H))-0.4E-4) 197,197,192
  192 IF (ITROT) 193,197,193
  193 PCP(2)=PCP(2)/(1.0+2.0*DHSTAR*WTMOL/(T*(GAMMA+1.0)))
      SENSE LIGHT 4
      ITROT=ITROT-1
      GO TO 49
C
C     CALCULATE PERFORMANCE PARAMETERS
C
  197 SP IMP=294.98*SQRTF((HC-SUM H)*1.98726E-3)
      P=PC/PCP(IADD)
      AW=(86.4579*T)/(P*WTMOL*14.696006*SP IMP)
      IF (IADD-2) 203,201,203
  201 AWT=AW
      CSTAR=32.174*PC*14.696006*AWT
  203 CF=32.174*SP IMP/CSTAR
      ARATIO=AW/AWT
      VACI=SP IMP+P*14.696006*AW
      VMACH=SP IMP/SQRTF(86.4579*GAMMA*T/WTMOL)
  207 ANS(2)=P
      ANS(3)=T
  209 HSUM=SUM H*1.98726
      CP=CPR*1.98726
      ANS(1)=PCP(IADD)
      ANS(15)=CSTAR
      WRITE TAPE 3,(ANS(I),I=1,454)
      NO FROZ=NO FROZ+1
      IF (MISSED) 451,223,451
  223 IADD=IADD+1
      IF (IADD-2) 1225,224,1225
  224 PCP(2)=((GAMMA+1.0)/2.0)**(GAMMA/(GAMMA-1.0))
      T LN=T LN+LOGF(2.0/(GAMMA+1.0))
 1225 IF (IADD-25) 225,225,451
  225 IF (PCP(IADD)) 451,451,227
```

```
  227 SENSE LIGHT 4
      GO TO 49
C
C     ERROR PRINT OUT
C
  305 WRITE OUTPUT TAPF 6,306,T,IADD
  306 FORMAT (17HLTHE TEMPERATURE=E12.4,26H K, IS OUT OF RANGE,POINT I5)
      IF (6000.0-T) 449,307,307
  307 IF (T-200.0) 449,308,308
  308 GO TO 41
  449 MISSED=1
      ITROT=0
      IF (SENSE LIGHT 4) 51,51
  451 WRITE TAPE 3, (G(I), I=1,8044)
      CALL CORE5
      RETURN
  309 WRITE OUTPUT TAPE 6,310,(COEFT(I,J),I=1,3),COEFT(6,J),COEFT(7,J)
  310 FORMAT (13H6THE SPECIES 3A6,29H HAS NO DATA IN THE INTERVAL 2F9.1)
      DO 1311 K = 1,15
      DO 1311 J = 1,90
 1311 COEFT(K,J) = COEFT1(K,J)
      GO TO 449
  311 WRITE OUTPUT TAPE 6,312, (COEFT(I,J),I=1,3),T
  312 FORMAT (13H6THE SPECIES 3A6,19H HAS NO DATA AT T= F9.1)
      GO TO 449
```

```
      SUBROUTINE  CORE4
C
C     CHAPMAN-JOUGUET DETONATIONS
C
C
      COMMON C
      EQUIVALENCE   (G(1),      C(1)),    (G(420),    C(420))
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),    C(874))
      EQUIVALENCE   (HSUM,      C(424)),  (SSUM,      C(425))
      EQUIVALENCE   (WTMOL,     C(426)),  (CP,        C(427))
      EQUIVALENCE   (DLMPT,     C(428)),  (DLMTP,     C(429))
      EQUIVALENCE   (GAMMA,     C(430)),  (ARATIO,    C(431))
      EQUIVALENCE   (VMACH,     C(432)),  (SP IMP,    C(433))
      EQUIVALENCE   (VACI,      C(434)),  (CF,        C(436))
      EQUIVALENCE   (RHOI,      C(437)),  (RHOVAC,    C(438))
      EQUIVALENCE   (RHO,       C(439))
      EQUIVALENCE   (T PI,      C(440)),  (PI I,      C(441))
      EQUIVALENCE   (EP PI,     C(442)),  (AW PI,     C(443))
      EQUIVALENCE   (T ETA,     C(445))
      EQUIVALENCE   (ETA I,     C(446)),  (EP ETA,    C(447))
      EQUIVALENCE   (AW ETA,    C(448)),  (T SIG,     C(450))
      EQUIVALENCE   (SIG I,     C(451)),  (EP SIG,    C(452))
      EQUIVALENCE   (AW SIG,    C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),   C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,     C(1472))
      EQUIVALENCE   (ACX,      C(1474)),   (ACF,     C(1475))
      EQUIVALENCE   (AMX,       C(1476)),   (AMF,      C(1477))
      EQUIVALENCE   (RHOX,      C(1478)),   (RHOF,    C(1479))
      EQUIVALENCE   (COEFX(1),    C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),    C(1500)),  (DX(20),    C(1519))
      EQUIVALENCE   (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),   C(1520)),  (MMLA(18), C(1537))
      EQUIVALENCE   (PROD(1),  C(1538)),  (PROD(3),    C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),  (SYSTM(15),   C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OF,     C(1556)),     (FPCT,   C(1557))
      EQUIVALENCE   (OOF,     C(1556))
      EQUIVALENCE   (PERCF,     C(1557)),      (EQUIV,     C(1558))
      EQUIVALENCE   (EQRAT,     C(1558))
      EQUIVALENCE                         (KASE,      C(1560))
      EQUIVALENCE   (KONT,   C(1561)),    (NF,          C(1562))
      EQUIVALENCE   (NO,          C(1563)), (NE,          C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (NOFROZ,     C(1566))
      EQUIVALENCE   (P1,        C(1567)),  (T1,          C(1568))
      EQUIVALENCE   (AM1,          C(1569)), (H1,          C(1570))
      EQUIVALENCE   (CON,         C(1571)), (ITR,         C(1572))
      EQUIVALENCE   (R,           C(1573)), (KODE,        C(1574))
      EQUIVALENCE   (JEAN,        C(1575)), (GAMF,      C(1585))
      EQUIVALENCE   (A1,    C(1576)), (A2,    C(1577)),  (A3,   C(1578))
      EQUIVALENCE   (A4,   C(1579)),    (A5,   C(1580)),   (A6,  C(1581))
      EQUIVALENCE   (A7,  C(1582)),  (A8,  C(1583)),   (A9,   C(1584))
      EQUIVALENCE   (UUS,         C(1586)),      (US,  C(1587))
      EQUIVALENCE   (PPP,      C(1588)),       (TTT,      C(1589))
      EQUIVALENCE   (TE,     C(1590)),       (TEM,     C(1591))
      EQUIVALENCE   (AMD,      C(1592)),       (UD,     C(1593))

      EQUIVALENCE    (AMOL(1),   C(1594)),    (AMOL(105),   C(1698))
      EQUIVALENCE (KD, C(1763)), (II, C(1764))
      EQUIVALENCE (MM, C(1765)), (IN, C(8046))
      EQUIVALENCE (ME, C(1769)), (KORE, C(8047))
      EQUIVALENCE   (BOX(1),      C(1771)), (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),      C(1786)), (BOF(15),   C(1800))
      EQUIVALENCE   (HX,          C(1801)), (HF,        C(1802))
      EQUIVALENCE   (VXPLS,       C(1803)), (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,       C(1805)), (VFMIN,     C(1806))
      EQUIVALENCE (ELMT(1), C(1807)), (ELMT(15), C(1821))
      EQUIVALENCE (LLMT(1), C(1807)), (LLMT(15), C(1821))
      EQUIVALENCE   (EN LN(1),  C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),  C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (HO(1),       C(2041)), (HO(90),    C(2130))
      EQUIVALENCE   (S(1),        C(2131)), (S(90),     C(2220))
      EQUIVALENCE   (X(1),        C(2221)), (X(20),     C(2240))
      EQUIVALENCE   (DELTA(1),  C(2241)), (DELTA(20), C(2260))
      EQUIVALENCE   (BO(1),       C(2261)), (BO(15),    C(2275))
      EQUIVALENCE   (PO,          C(2276)), (HSUBO,     C(2277))
      EQUIVALENCE   (SO,          C(2278)), (T LN,      C(2279))
      EQUIVALENCE   (T,           C(2280)), (AAY LN,    C(2281))
      EQUIVALENCE   (AAY,         C(2282)), (CPSUM,     C(2283))
      EQUIVALENCE   (HC,          C(2284)), (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),      C(2286)), (PCP(25),   C(2310))
      EQUIVALENCE   (DATUM(1),  C(2311)), (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,          C(2314)), (TC,        C(2315))
      EQUIVALENCE   (IPROB,       C(2316)), (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,         C(2318)), (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,        C(2320)), (IPROD,     C(2321))
      EQUIVALENCE   (IDID,        C(2322)), (LDRUM,     C(2323))
      EQUIVALENCE   (IDRM,        C(2323)), (KDRUM,     C(2324))
      EQUIVALENCE   (L,           C(2325)), (L1,        C(2326))
      EQUIVALENCE   (M,           C(2327)), (M1,        C(2328))
      EQUIVALENCE   (N,           C(2329)), (IQ,        C(2330))
      EQUIVALENCE   (IQ1,         C(2331)), (IQ2,       C(2332))
      EQUIVALENCE   (IQ3,         C(2333)), (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,        C(2335)), (IUSE,      C(2335))
      EQUIVALENCE   (IADD,        C(2336)), (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,       C(2338)), (P,         C(2339))
      EQUIVALENCE   (IDEBUG,      C(2340)), (IFROZ,     C(2341))
      EQUIVALENCE   (COEFT1(1),   C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),   (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
      EQUIVALENCE   (TITLE(1),     C(8055)), (TITLE(315), C(8369))
      EQUIVALENCE(A(1), C(8578)),  (A(690), C(9267))
C
      DIMENSION   G(20,21),    A(15,90),    EN(90),      EN LN(90)
      DIMENSION   DEL N(90),   HO(90),      S(90),       X(20)
      DIMENSION   DELTA(20),   BO(15),      PCP(25),     PROD(3)
      DIMENSION   COEFX(20),   DX(20),      FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),    DATA(23),    DATUM(3),    FORMLA(18)
      DIMENSION   BOX(15),     BOF(15),     ANS(454),    SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),      ATOM(101,3)
C
C
```

```
C     CORE LOAD 4    DETONATION VELOCITIES
      IF(JEAN-101)100,101,100
  100 WRITE OUTPUT TAPE 6,2
    2 FORMAT (38H1    DETONATION VELOCITY    CALCULATIONS)
      PPP=15.0
      CON=(ACF+OOF*ACX)/(1.0+OOF)
      AM1=AMX*AMF*(1.0+OOF)/(AMX+OOF*AMF)
      WRITE OUTPUT TAPE 6,102,KODE
  102 FORMAT (4X,5HKODE=I1)
      PCP(1)=1.0/PPP
      PCP(2)=0.0
      R=1.98726
      TTT=0.0
      H1=HSUBO*R
      P1=PC
      T1=TC
      PC=PC*14.696006
      ITR=0
      JEAN=101
   20 HSUBO=H1/R+.75*T1/AM1*PPP
   21 KORE  =0
      RETURN
  101 DO 1101 J= 1,454
 1101 ANS(J) = ANSLAB(J)
      GAM=GAMMA
      IF(KODE)91,92,91
   91 GAMMA=GAMMA*(1.0+DLMPT)
   92 PPP=ANS(2)/P1
      TTT=ANS(3)/T1
      E=PPP
      EE=TTT
      IF(ITR)201,200,201
  200 TEMM=WTMOL/AM1
      II=0
      WRITE OUTPUT TAPE 6,203,II,PPP,TTT
      DO 202 II=1,7
      TEM=TEMM/TTT*GAMMA
      PPPP=(1.0+GAMMA)/(2.0*TEM)*
     2(1.0+SQRTF(1.0-4.0*TEM/(1.0+GAMMA)**2))
      TE=TEM/GAMMA*PPPP
      TTTT=EE-.75*R/(AM1*CP)*E+GAMMA*R/(2.*AM1*CP)*((TE**2-1.0)/TE)*PPPP
      WRITE OUTPUT TAPE 6,203,II,PPPP,TTTT
  203 FORMAT(I5,2E20.8)
      IF(ABSF(PPPP-PPP)-.1)205,205,206
  206 PPP=PPPP
      TTT=TTTT
  202 CONTINUE
  205 PCP(1)=T1*TTTT
      PC=P1*PPPP
      TC=0.0
      IPROB=3
      ITR=1
      GAMMA=GAM
      GO TO 21
  201 TEMM=PPP/TTT*WTMOL/AM1
      TEM=(1.0-GAMMA*(TEMM-1.0))
      A11=1.0/PPP-GAMMA*TEMM*(1.0+DLMPT)
      A12=GAMMA*TEMM*(1.0-DLMTP)
      A21=GAMMA/2.0*(DLMPT+TEMM**2*(2.0+DLMPT))-DLMTP
      HAL=GAMMA/2.0*(TEMM**2+1.0)

      A22=HAL*(DLMTP-1.0)-WTMOL*CP/R
      B1=1.0/PPP-TEM
      B2=WTMOL/(R*ANS(3))*(HSUM-H1)-GAMMA/2.0*(TEMM**2-1.0)
      ASSIGN 51 TO JJ
   50 EEM=A11*A22-A21*A12
      X1=(B1*A22-B2*A12)/EEM
      X2=(A11*B2-A21*B1)/EEM
      GO TO JJ,(51,52,53,      59)
   51 TE=ABSF(X1)
      TEM=ABSF(X2)
      IF(TE-.4)94,94,95
   94 IF(TEM-.4)96,96,95
   96 ALAM=1.0
      GO TO 97
   95 IF(TE-TEM)93,93,98
   93 HAL=TEM
      GO TO 99
   98 HAL=TE
   99 ALAM=.4/HAL
   97 PPPP=PPP*EXPF(X1*ALAM)
      TTTT=TTT*EXPF(X2*ALAM)
  301 US=91.18496 *SQRTF(GAMMA*ANS(3)/WTMOL)
      UD=TEMM*US
      PCP(1)=T1*TTTT
      PC=P1*PPPP
      TC=0.0
      IPROB=3
      TE=WTMOL/AM1
      TEM=PPPP/TTTT*TE
      E=X1**2+X2**2
      EE=SQRTF(E)
      WRITE OUTPUT TAPE 6,10,ITR
   10 FORMAT (21H0    ITERATION NUMBER=I2,10X,3HOLD,17X,3HNEW//)
      WRITE OUTPUT TAPE 6,30,PPP,PPPP,TTT,TTTT,TEMM,TEM,X1,X2,US,UD,E
     2,EE
   30 FORMAT(6X,4HP/P1,10X,1H=2E20.8/6X,4HT/T1,10X,1H=2E20.8/6X,8HRHO/RH
     1O1,6X,1H=2E20.8/6X,11HDEL LN P/P1,3X,1H=E20.8/6X,11HDEL LN T/T1,3X
     2,1H=E20.8/6X,2HUS,12X,1H=E20.8/6X,2HUD,12X,1H=E20.8/6X,1HE,13X,1H=
     3E20.8/6X,13HSQR ROOT OF E,1X,1H=E20.8)
      PPP=PPPP
      TTT=TTTT
      IF(ABSF(X1)-.5E-05)11,11,12
   11 IF(ABSF(X2)-.5E-05)13,13,12
   12 IF(ITR-10)14,13,13
   14 ITR=ITR+1
      GAMMA=GAM
      GO TO 21
   13 JEAN=10
      P=PPP*P1
      T=TTT*T1
      US=91.18496 *SQRTF(GAMMA*T/WTMOL)
      UD=TEM*US
      WRITE OUTPUT TAPE 6,31
   31 FORMAT (17H1    FINAL ANSWERS//)
      WRITE OUTPUT TAPE 6,32,PPP,TTT,TE,TEM,P,T,WTMOL,P1,T1,AM1,US,UD
     2,CON
   32 FORMAT (6X,4HP/P1,10X,1H=E20.8/6X,4HT/T1,10X,1H=E20.8/6X,4HM/M1,10
     2X,1H=E20.8/6X,8HRHO/RHO1,6X,1H=E20.8/6X,1HP,13X,1H=E20.8/6X,1HT,13
     3X,1H=E20.8/6X,1HM,13X,1H=E20.8/6X,2HP1,12X,1H=E20.8/6X,2HT1,12X,1H
     4=E20.8/6X,2HM1,12X,1H=E20.8/6X,2HUS,12X,1H=E20.8/6X,2HUD,12X,1H=E2
```

```
    50.8/6X,2HCP,12X,1H=E20.8)
      IF(CON)41,40,41
   41 GAMF=CON/(CON-R/AM1)
      AMD=UD/(91.18496*SQRTF(GAMF*T1/AM1))
      WRITE OUTPUT TAPE 6,42,GAMF,AMD
   42 FORMAT (6X,7HGAMMA F,7X,1H=E20.8/6X,2HMD,12X,1H=E20.8)
      GO TO 150
   40 GAMF=0.0
      AMD=0.0
  150 FEM=.5*(2.0+DLMPT)
      TEMM=.5*(DLMTP-1.0)
      WRITE OUTPUT TAPE 6,55
   55 FORMAT (17H0   DERIVATIVE OF,12X,4HLN P,13X,4HLN T,13X,5HLN UD/4X,
     22HBY)
      B1=1.0/PPP-GAMMA*TEM
      B2=GAMMA*  TEM**2
      ASSIGN 53 TO JJ
      GO TO 50
   53 CASE1=(FEM*X1+TEMM*X2-1.0)*UD
      X1=X1-1.0
      WRITE OUTPUT TAPE 6,81,X1,X2,CASE1
   81 FORMAT (6X,12HLNP1 AT T1,G,7X,1H=3E17.8)
      A1=X1
      A2=X2
      A3=CASE1
      B1=GAMMA*TEM
      B2=-B1*TEM-WTMOL*CON/R/TTT
      ASSIGN 59 TO JJ
      GO TO 50
   59 CASE4=(FEM*X1+TEMM*X2+1.0)*UD
      X2=X2-1.0
      WRITE OUTPUT TAPE 6,84,X1,X2,CASE4
   84 FORMAT(6X,16HLNT1 AT P1,H1,M1,3X,1H=3E17.8)
      A4=X1
      A5=X2
      A6=CASE4
      B1=0.0
      B2=-WTMOL/(R*T)
      ASSIGN 52 TO JJ
      GO TO 50
   52 X1=X1*1000.0
      X2=X2*1000.0
      CASE5=(FEM*X1+TEMM*X2)*UD
      WRITE OUTPUT TAPE 6,85,X1,X2,CASE5
   85 FORMAT (6X,20HH1    AT T1,P1,M1    =3E17.8)
      A7=X1
      A8=X2
      A9=CASE5
      GAMMA=GAM
      IPROB=1
      UUS=91.18496*SQRTF(GAMF*T1/AM1)
      WRITE TAPE 3,(G(I),I=1,8044)
      CALL OUT
      KORE=1
      RETURN
```

```
      SUBROUTINE OUT
C
      COMMON C
      EQUIVALENCE   (G(1),      C(1)),    (G(420),    C(420))
      EQUIVALENCE   (ANS(1), C(421)),  (ANS(454),   C(874))
      EQUIVALENCE   (HSUM,      C(424)),  (SSUM,      C(425))
      EQUIVALENCE   (WTMOL,     C(426)),  (CP,        C(427))
      EQUIVALENCE   (DLMPT,     C(428)),  (DLMTP,     C(429))
      EQUIVALENCE   (GAMMA,     C(430)),  (ARATIO,    C(431))
      EQUIVALENCE   (VMACH,     C(432)),  (SP IMP,    C(433))
      EQUIVALENCE   (VACI,      C(434)),  (CF,        C(436))
      EQUIVALENCE   (RHOI,      C(437)),  (RHOVAC,    C(438))
      EQUIVALENCE   (RHO,       C(439))
      EQUIVALENCE   (T PI,      C(440)),  (PI I,      C(441))
      EQUIVALENCE   (EP PI,     C(442)),  (AW PI,     C(443))
      EQUIVALENCE   (T ETA,     C(445))
      EQUIVALENCE   (ETA I,     C(446)),  (EP ETA,    C(447))
      EQUIVALENCE   (AW ETA,    C(448)),  (T SIG,     C(450))
      EQUIVALENCE   (SIG I,     C(451)),  (EP SIG,    C(452))
      EQUIVALENCE   (AW SIG,    C(453))
      EQUIVALENCE   (ANSLAB(1), C(875)), (ANSLAB(454), C(1328))
      EQUIVALENCE   (FORM(1),   C(1329)), (FORM(15),  C(1343))
      EQUIVALENCE   (DATA(1),  C(1359)),  (DATA(23),  C(1381))
      EQUIVALENCE   (MDATA(1),  C(1359)),  (MDATA(23), C(1381))
      EQUIVALENCE   (EN(1),   C(1382)),  (EN(90),   C(1471))
      EQUIVALENCE   (ISYS,      C(1472))
      EQUIVALENCE   (ACX,       C(1474)),   (ACF,      C(1475))
      EQUIVALENCE   (AMX,         C(1476)),   (AMF,       C(1477))
      EQUIVALENCE   (RHOX,      C(1478)),   (RHOF,     C(1479))
      EQUIVALENCE   (COEFX(1),     C(1480)),  (COEFX(20),  C(1499))
      EQUIVALENCE   (DX(1),     C(1500)),  (DX(20),    C(1519))
      EQUIVALENCE   (FORMLA(1),  C(1520)),  (FORMLA(18),  C(1537))
      EQUIVALENCE   (MMLA(1),   C(1520)),  (MMLA(18), C(1537))
      EQUIVALENCE   (PROD(1),  C(1538)),  (PROD(3),   C(1540))
      EQUIVALENCE   (SYSTM(1),  C(1541)),  (SYSTM(15),   C(1555))
      EQUIVALENCE   (MTSYS(1), C(1541)), (MTSYS(15),  C(1555))
      EQUIVALENCE   (OOF,     C(1556))
      EQUIVALENCE   (OF,      C(1556)),      (FPCT,   C(1557))
      EQ'JIVALENCE   (PERCF,     C(1557)),      (EQUIV,     C(1558))
      EQUIVALENCE   (EQRAT,     C(1558))
      EQUIVALENCE                          (KASE,      C(1560))
      EQUIVALENCE   (KONT,   C(1561)),     (NF,         C(1562))
      EQUIVALENCE   (NO,        C(1563)), (NE,         C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (NOFROZ,    C(1566))
      EQUIVALENCE   (P1,        C(1567)),  (T1,         C(1568))
      EQUIVALENCE   (AM1,         C(1569)), (H1,         C(1570))
      EQUIVALENCE   (CON,       C(1571)), (ITR,        C(1572))
      EQUIVALENCE   (R,         C(1573)), (KODE,       C(1574))
      EQUIVALENCE   (JEAN,      C(1575)), (GAMF,     C(1585))
      EQUIVALENCE   (A1,    C(1576)), (A2,   C(1577)),  (A3,   C(1578))
      EQUIVALENCE   (A4,   C(1579)),   (A5,   C(1580)),   (A6,  C(1581))
      EQUIVALENCE   (A7,  C(1582)),  (A8,  C(1583)),   (A9,   C(1584))
      EQUIVALENCE   (UUS,         C(1586)),     (US,  C(1587))
      EQUIVALENCE   (PPP,     C(1588)),       (TTT,      C(1589))
      EQUIVALENCE   (TE,     C(1590)),       (TEM,     C(1591))
      EQUIVALENCE   (AMD,     C(1592)),       (UD,    C(1593))
      EQUIVALENCE (KD, C(1763)), (II, C(1764))
      EQUIVALENCE (MM, C(1765)), (IN, C(8046))
      EQUIVALENCE (ME, C(1769))

      EQUIVALENCE   (BOX(1),    C(1771)), (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),    C(1786)), (BOF(15),   C(1800))
      EQUIVALENCE   (HX,        C(1801)), (HF,        C(1802))
      EQUIVALENCE   (VXPLS,     C(1803)), (VXMIN,     C(1804))
      EQUIVALENCE   (VFPLS,     C(1805)), (VFMIN,     C(1806))
      EQUIVALENCE   (EN LN(1),  C(1861)), (EN LN(90), C(1950))
      EQUIVALENCE   (DEL N(1),  C(1951)), (DEL N(90), C(2040))
      EQUIVALENCE   (HO(1),     C(2041)), (HO(90),    C(2130))
      EQUIVALENCE   (S(1),      C(2131)), (S(90),     C(2220))
      EQUIVALENCE   (X(1),      C(2221)), (X(20),     C(2240))
      EQUIVALENCE   (DELTA(1),  C(2241)), (DELTA(20), C(2260))
      EQ'JIVALENCE   (BO(1),     C(2261)), (BO(15),    C(2275))
      EQUIVALENCE   (PO,        C(2276)), (HSUBO,     C(2277))
      EQUIVALENCE   (SO,        C(2278)), (T LN,      C(2279))
      EQUIVALENCE   (T,         C(2280)), (AAY LN,    C(2281))
      EQUIVALENCE   (AAY,       C(2282)), (CPSUM,     C(2283))
      EQUIVALENCE   (HC,        C(2284)), (TC LN,     C(2285))
      EQUIVALENCE   (PCP(1),    C(2286)), (PCP(25),   C(2310))
      EQUIVALENCE   (DATUM(1),  C(2311)), (DATUM(3),  C(2313))
      EQUIVALENCE   (PC,        C(2314)), (TC,        C(2315))
      EQUIVALENCE   (IPROB,     C(2316)), (IFIXT,     C(2317))
      EQUIVALENCE   (IHS,       C(2318)), (ICOND,     C(2319))
      EQUIVALENCE   (ISYM,      C(2320)), (IPROD,     C(2321))
      EQUIVALENCE   (IDID,      C(2322)), (LDRUM,     C(2323))
      EQUIVALENCE   (IDRM,      C(2323)), (KDRUM,     C(2324))
      EQUIVALENCE   (L,         C(2325)), (L1,        C(2326))
      EQUIVALENCE   (M,         C(2327)), (M1,        C(2328))
      EQUIVALENCE   (IQ1,       C(2331)), (IQ2,       C(2332))
      EQUIVALENCE   (N,         C(2329)), (IQ,        C(2330))
      EQUIVALENCE   (IQ3,       C(2333)), (KMAT,      C(2334))
      EQUIVALENCE   (IMAT,      C(2335)), (IUSE,      C(2335))
      EQUIVALENCE   (IADD,      C(2336)), (ITNUMB,    C(2337))
      EQUIVALENCE   (ITAPE,     C(2338)), (P,         C(2339))
      EQUIVALENCE   (IDEBUG,    C(2340)), (IFROZ,     C(2341))
      EQUIVALENCE   (COEFT1(1),  C(3692)), (COEFT1(1350), C(5041))
      EQUIVALENCE   (COEFT2(1), C(5042)), (COEFT2(1350), C(6391))
      EQUIVALENCE   (COEFT(1),  C(6392)),  (COEFT(1350), C(7741))
      EQUIVALENCE   (ATOM(1),  C(7742)), (ATOM(303), C(8044))
      EQUIVALENCE   (MATOM(1),  C(7742)), (MATOM(303),  C(8044))
      EQUIVALENCE   (TITLE(1),    C(8055)), (TITLE(315), C(8369))
      EQUIVALENCE (ELMT(1), C(1807)), (ELMT(15), C(1821))
      EQUIVALENCE TLLMT(1), C(1807)), (LLMT(15), C(1821))
      EQUIVALENCE (AMOL(1), C(9268)), (AMOL(1170),  C(10437))
      EQUIVALENCE(A(1), C(8578)),  (A(690), C(9267))
C
      DIMENSION   G(20,21),                 EN(90),     EN LN(90)
      DIMENSION   DEL N(90),  HO(90),       S(90),      X(20)
      DIMENSION   DELTA(20),  BO(15),       PCP(25),    PROD(3)
      DIMENSION   COEFX(20),  DX(20),       FORM(15)
      DIMENSION COEFT1(15,90) , COEFT2(15,90)
      DIMENSION   ELMT(15),   DATA(23),     DATUM(3),   FORMLA(18)
      DIMENSION   BOX(15),    BOF(15),      ANS(454),   SYSTM(15)
      DIMENSION LLMT(15),MTSYS(15),MDATA(23)
      DIMENSION   ANSLAB(454),   COEFT(15,90)
      DIMENSION   MATOM(101,3),      ATOM(101,3)
      DIMENSION TITLE(3,105),              A(15,46)
      DIMENSION AMOL(13,90)
C
C
    2 FORMAT (9HOCASE NO.I5,F8.2,F8.2)
```

```
    3 FORMAT (1H0,64X,52HWT FRACTION  ENTHALPY   STATE  TEMP    HEAT CAP
     2ACITY/25X,16HCHEMICAL FORMULA,24X,10H(SEE NOTE),4X,7HCAL/MOL,12X,
     35HDEG K,5X,13HCAL/MOL-DEG K)
    4 FORMAT (1H0,84X,46HWT FRACTION  ENTHALPY   STATE  TEMP       CP
     2        25X,16HCHEMICAL FORMULA,44X,10H(SEE NOTE),4X,7HCAL/MOL,
     3        10X,5HDEG K)
    5 FORMAT(1H+,63X,F9.5,F12.3,4X,A1,F10.2,F11.4)
    6 FORMAT(1H+,83X,F9.5,F12.3,4X,A1,F10.2,F11.4)
    7 FORMAT (1H0,30X,4HO/F=F9.6,15H, PERCENT FUEL=F8.4,20H, EQUIVALENCE
     1 RATIO=F7.4)
   20 FORMAT      (43X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS)
   21 FORMAT (43X,45HCALCULATED USING SPECIFIC HEAT RATIO AS GAMMA)
   22 FORMAT (1H0,24HTHERMODYNAMIC PROPERITES/27X,12HUNBURNED GAS, 5X,10
     2HBURNED GAS)
   23 FORMAT (1X,6HP, ATM,20X,F12.5,3X,F12.5)
   24 FORMAT (1X,8HT, DEG K,18X,F12.2,3X,F12.1)
   25 FORMAT (1X,9HH, CAL/G ,17X,F12.1,3X,F12.1)
   26 FORMAT (1X,15HS, CAL/G-DEG K ,26X,F12.4)
   27 FORMAT (1X,11HM, MOL. WT.15X,F12.3,3X,F12.3)
   28 FORMAT (1X,16HCP, CAL/G-DEG K ,10X,F12.4,3X,F12.4)
   29 FORMAT (1X,12H(DLNM/DLNP)T,14X,F12.5,3X,F12.5)
   30 FORMAT (1X,12H(DLNM/DLNT)P,14X,F12.4,3X,F12.4)
   31 FORMAT (1X,5HGAMMA,21X,F12.4,3X,F12.4)
   32 FORMAT (1X,9HUS, M/SEC,17X,F12.1,3X,F12.1)
   33 FORMAT(1H0/1X,40HBURNED GAS COMPOSITION IN MOLE FRACTIONS//)
   34 FORMAT (1H0/1X,21HDETONATION PARAMETERS,
     22X,27H(UD IN M/SEC, H1 IN KCAL/G))
   35 FORMAT (1H0,4HP/P1,4X,1H=F7.3,5X,21H(DL(P/P1)/DLP1)T1,H1=F8.5,5X,1
     28H(DL(P/P1)/DLT1)P1=F8.5,5X,20H(DL(P/P1)/DH1)P1,T1=F8.5)
   36 FORMAT ( 1X,4HT/T1,4X,1H=F7.3,5X,21H(DL(T/T1)/DLP1)T1,H1=F8.5,5X,1
     18H(DL(T/T1)/DLT1)P1=F8.5,5X,20H(DL(T/T1)/DH1)P1,T1=F8.5)
   37 FORMAT (1X,4HM/M1,4X,1H=F7.4)
   38 FORMAT (1X,9HRHO/RHO1=F7.4)
   39 FORMAT (1X,9HMACH NO.=F7.4)
   40 FORMAT (1X,9HUD       =F7.1,5X,16H(D UD/DLP1)T1,H1,4X,1H=F8.2,5X,13
     1H(D UD/DLT1)P14X,1H=F8.2,5X,15H(D UD/DH1)P1,T1,4X,1H=F8.2)
 1000 WRITE OUTPUT TAPE 6,18
   18 FORMAT (1H1)
  552 REWIND 3
  300 READ TAPE 3,(ANS(I),I=1,454)
      HAL=P1*14.696006
      I=1
      J=38
      DO 350 JJ=1,N
      AMOL(1,I)=ANS(J)
      J=J+4
  350 I=I+1
      WRITE OUTPUT TAPE 6,20
      IF(KODE)351,352,351
  351 WRITE OUTPUT TAPE 6,21
  352 CONTINUE
B     ZERO=000000000000
  106 J=34
      DO 104 I=1,N
      DO 105 II=1,3
      KK=J+II
  105 TITLE(II,I)=ANS(KK)
  104 J=J+4
      ASSIGN 90 TO JEAN
   92 WRITE OUTPUT TAPE 6,2,KASE,HAL,T1

      GO TO JEAN,(90,91)
   90 IF(KD)93,94,93
   94 WRITE OUTPUT TAPE 6,3
      GO TO 97
   93 WRITE OUTPUT TAPE 6,4
   97 IF(NF)451,450,451
  451 DO 100 I=1,NF
      II=I
      MM=15
      CALL SPEC
      IF(KD)401,400,401
  400 WRITE OUTPUT TAPE 6,5,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
      GO TO 100
  401 WRITE OUTPUT TAPE 6,6,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
  100 CONTINUE
  450 IF(NO)453,452,453
  453 DO 101 I=1,NO
      II=I
      MM=0
      CALL SPEC
      IF(KD)411,410,411
  410 WRITE OUTPUT TAPE 6,5,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
      GO TO 101
  411 WRITE OUTPUT TAPE 6,6,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
  101 CONTINUE
  452 CONTINUE
      WRITE OUTPUT TAPE 6,7,OOF,PERCF,EQUIV
      WRITE OUTPUT TAPE 6,22
      WRITE OUTPUT TAPE 6,23,P1,P
      WRITE OUTPUT TAPE 6,24,T1,T
      WRITE OUTPUT TAPE 6,25,H1,ANS(4)
      WRITE OUTPUT TAPE 6,26,ANS(5)
      WRITE OUTPUT TAPE 6,27,AM1,ANS(6)
      WRITE OUTPUT TAPE 6,28,CON,ANS(7)
      WRITE OUTPUT TAPE 6,29,ZERO,ANS(8)
      WRITE OUTPUT TAPE 6,30,ZERO,ANS(9)
      WRITE OUTPUT TAPE 6,31,GAMF,ANS(10)
      WRITE OUTPUT TAPE6,32,UUS,US
      WRITE OUTPUT TAPE 6,33
      IN=1
      ME=2
      CALL COMP
      WRITE OUTPUT TAPE 6,34
      WRITE OUTPUT TAPE 6,35,PPP,A1,A4,A7
      WRITE OUTPUT TAPE 6,36,TTT,A2,A5,A8
      WRITE OUTPUT TAPE 6,40,UD,A3,A6,A9
      WRITE OUTPUT TAPE 6,37,TE
      WRITE OUTPUT TAPE 6,38,TEM
      WRITE OUTPUT TAPE 6,39,AMD
  207 WRITE OUTPUT TAPE 6,16
   16 FORMAT (1H0,30X,16HINPUT, G-ATOMS/G//)
      IF(NE-8)80,80,81
   80 KK=1
      KKK=NE
      LOOP=1
      GO TO 82
   81 KK=1
      KKK=8
      LOOP=2
   82 DO 85 J=1,LOOP
```

```
      WRITE OUTPUT TAPE 6,11,(ELMT(I),I=KK,KKK)
   11 FORMAT (11X,8(6X,A2,7X))
      WRITE OUTPUT TAPE 6,12,(BOF (I),I=KK,KKK)
   12 FORMAT (5H FUEL,6X,8E15.7)
      WRITE OUTPUT TAPE 6,13,(BOX (I),I=KK,KKK)
   13 FORMAT (8H OXIDANT,3X,8E15.7)
      WRITE OUTPUT TAPE 6,14,(BO  (I),I=KK,KKK)
   14 FORMAT (11H PROPELLANT,8E15.7)
      IF (LOOP-1) 86,85,86
   86 KK=9
      KKK=NE
      WRITE OUTPUT TAPE 6,15
   15 FORMAT(1H0)
   85 CONTINUE
      ASSIGN 91 TO JEAN
      GO TO 92
   91 WRITE OUTPUT TAPE 6,119
  119 FORMAT (6H0NOTE.,2X,71HWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND
     1OF OXIDANT IN TOTAL OXIDANTS)
      RETURN

      SUBROUTINE ONCE (N,M)
C
C     OUTPUTS ODD PRODUCTS
C
C
      COMMON C
      EQUIVALENCE   (TITLE(1),    C(8055)), (TITLE(315), C(8369))
      DIMENSION M(105),TITLE(3,105) ,TEM(10),FMT(3)
      WRITE OUTPUT TAPE 6,1
B     FMT(1)=740130207360
B     FMT(3)=210634606060
B     TEM(1)=606001677302
B     TEM(2)=600104677302
B     TEM(3)=600207677302
B     TEM(4)=600400677302
B     TEM(5)=600503677302
B     TEM(6)=600606677302
B     TEM(7)=600711677302
B     TEM(8)=601102677302
B     TEM(9)=010005677302
B     TEM(10)=010110677302
      K=0
      KK=10
      DO 10 I=1,N
      J=M(I)
      IF(I-KK) 20,20,21
   20 K=K+1
      GO TO 5
   21 K=1
      KK=KK+10
      WRITE OUTPUT TAPE 6,1
    1 FORMAT (1H )
    5 FMT(2)=TEM(K)
      WRITE OUTPUT TAPE 6,FMT,TITLE(2,J),TITLE(3,J)
   10 CONTINUE
      RETURN

      SUBROUTINE SPEC
C
C     OUTPUTS FUEL AND OXIDANT FROM SUBROUTINE INPUT
C
C
      COMMON C
      EQUIVALENCE (KONT, C(1763))
      EQUIVALENCE (I, C(1764)), (M,C(1765))
      EQUIVALENCE (A(1),  C(8578)),  (A(690),  C(9267))
      EQUIVALENCE (ELMT(1),  C(1807)), (ELMT(15),  C(1821))
      DIMENSION A(15,46),TEM(5),ANAME(5),ELMT(15)
      DIMENSION II(5)
   55 FORMAT (10X,4HFUEL)
   66 FORMAT (10X,7HOXIDANT)
      IF (M ) 2,1,2
    1 WRITE OUTPUT TAPE 6,66
      GO TO 3
    2 WRITE OUTPUT TAPE 6,55
    3 K=0
      DO 11 J=1,15
      KK=I+M
      IF(A(J,KK))12,11,12
   12 K=K+1
      TEM(K)=A(J,KK)
      ANAME(K)=ELMT(J)
      II(K)=TEM(K)
   11 CONTINUE
      IF(KONT)21,20,21
   20 WRITE OUTPUT TAPE 6,4,(ANAME(I),II(I),I=1,K)
    4 FORMAT(1H+,18X,5(A2,I2,5X))
      GO TO 13
   21 WRITE OUTPUT TAPE 6,5,(ANAME(I),TEM(I),I=1,K)
    5 FORMAT (1H+,18X,5(A2,F8.5,3X))
   13 RETURN
```

```
      SUBROUTINE COMP
C
C     OUTPUTS COMPOSITION
C
C
      COMMON C
      EQUIVALENCE (AMOL(1),  C(9268)),  (AMOL(1170),  C(10437))
      EQUIVALENCE (NANA, C(1768)), (IN, C(8046))
      EQUIVALENCE (ME, C(1769)), (N, C(2329))
      EQUIVALENCE   (TITLE(1),    C(8055)), (TITLE(315), C(8369))
      EQUIVALENCE   (MTITLE(1), C(8055)),  (MTITLE(315),   C(8369))
      EQUIVALENCE (OMIT,MOMIT)
      DIMENSION              TITLE(3,105),IOMIT(105),ILESS(105)
      DIMENSION AMOL(13,90)
      DIMENSION FMT(4),TEM(4)
      DIMENSION MTITLE (3,105)
    1 FORMAT (1X,2A6,2X,13F9.5)
    3 FORMAT (1H0,   118HADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT W
     1HOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDI
     2TIONS//)
    4 FORMAT (1H0,    59HPRODUCTS WHICH WERE INTENTIONALLY OMITTEC FROM
     1CALCULATIONS//)
B     OMIT=464431636060
B     TEM(1)=606007677302
B     TEM(2)=600306677302
B     TEM(3)=600604677302
B     TEM(4)=601102677302
B     FMT(1)=740130207360
B     FMT(3)=210673261033
B     FMT(4)=053460606060
      K=0
      KK=4
      IOM=0
      ILE=0
      IF(ME-1)61,60,61
   61 WRITE OUTPUT TAPE 6,44
   60 II=0
      DO 9 I=1,N
      IF (MTITLE(1,I)-MOMIT) 10,100,10
  100 IOM=IOM+1
      IOMIT(IOM)=I
      GO TO 9
   10 DO 11 J=1,IN
      IF(AMOL(J,I)-.5E-05)11,12,12
   11 CONTINUE
      ILE=ILE+1
      ILESS(ILE)=I
      GO TO 9
   12 IF(ME-1)51,50,51
   50 WRITE OUTPUT TAPE 6,1 ,TITLE(2,I),TITLE(3,I),(AMOL(JJ,I),JJ=1,IN)
      GO TO 9
   51 II=II+1
      IF(II-KK)200,200,201
  200 K=K+1
      GO TO 5
  201 K=1
      KK=KK+4
      WRITE OUTPUT TAPE 6,44
   44 FORMAT (1H )
    5 FMT(2)=TEM(K)

      WRITE OUTPUT TAPE 6,FMT,TITLE(2,I),TITLE(3,I),AMOL(1,I)
    9 CONTINUE
      IF(ILE) 21,20,21
   21 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,3
      CALL ONCE (ILE,ILESS)
   20 IF(IOM) 31,30,31
   31 WRITE OUTPUT TAPE 6,44
      WRITE OUTPUT TAPE 6,4
      CALL ONCE (IOM,IOMIT)
   30 RETURN
```

```
      SUBROUTINE  CORE5
C
C     OUTPUT ROUTINE
C
C
      COMMON C
      EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),    C(874))
      EQUIVALENCE   (PERCF,    C(1557)),     (EQUIV,    C(1558))
      EQUIVALENCE   (OOF,      C(1556))
      EQUIVALENCE (KODE,     C(1559)),    (KASE,       C(1560))
      EQUIVALENCE    (KONT,   C(1561)),     (NF,          C(1562))
      EQUIVALENCE   (NO,          C(1563)), (NE,          C(1564))
      EQUIVALENCE   (NOEQ, C(1565))
      EQUIVALENCE   (NOFROZ,     C(1566))
      EQUIVALENCE (KD, C(1763)), (II, C(1764))
      EQUIVALENCE (MM, C(1765))
      EQUIVALENCE (LEN, C(1766)), (MAY, C(1767))
      EQUIVALENCE (NANA, C(1768)), (ME, C(1769))
      EQUIVALENCE (LOOP, C(1770)), (KTAPE, C(8045))
      EQUIVALENCE   (BOX(1),     C(1771)), (BOX(15),   C(1785))
      EQUIVALENCE   (BOF(1),     C(1786)), (BOF(15),   C(1800))
      EQUIVALENCE   (BO(1),      C(2261)), (BO(15),    C(2275))
      EQUIVALENCE   (IPROB,      C(2316)), (IFIXT,     C(2317))
      EQUIVALENCE   (N,          C(2329)), (IQ,        C(2330))
      EQUIVALENCE (IN, C(8046))
      EQUIVALENCE (KK, C(8048)), (KKK, C(8049))
      EQUIVALENCE    (TITLE(1),     C(8055)), (TITLE(315), C(8369))
      EQUIVALENCE (ELMT(1), C(1807)), (ELMT(15), C(1821))
      EQUIVALENCE (PAR(1),  C(8370)), (PAR(208),  C(8577))
      EQUIVALENCE(A(1), C(8578)),  (A(690), C(9267))
      EQUIVALENCE (AMOL(1),  C(9268)),  (AMOL(1170),  C(10437))
      EQUIVALENCE (DER(1), C(10438)),  (DER(169), C(10606))
      DIMENSION         TITLE(3,105),PAR(13,16),DER(13,13),
     2             A(15,46),ELMT(15)
     3,ANS(454)
      DIMENSION BOX(15),BOF(15),BO(15)
      DIMENSION AMOL(13,90)
      DIMENSION          ASOL(13)
B     EXIT=256731636060
    2 FORMAT (9HOCASE NO.I5,F8.1,F7.3)
    3 FORMAT (1H0,64X,46HWT FRACTION  ENTHALPY   STATE  TEMP    DENSITY/
     225X,16HCHEMICAL FORMULA,24X,10H(SEE NOTE),4X,7HCAL/MOL,10X,
     35HDEG K,4X,4HG/CC)
    4 FORMAT (1H0,84X,46HWT FRACTION  ENTHALPY   STATE  TEMP    DENSITY/
     2          25X,16HCHEMICAL FORMULA,44X,10H(SEE NOTE),4X,7HCAL/MOL,
     3          8X,5HDEG K,4X,4HG/CC)
    5 FORMAT(1H+,63X,F9.5,F12.3,4X,A1,F10.2,F11.6)
    6 FORMAT(1H+,83X,F9.5,F12.3,4X,A1,F10.2,F11.6)
    7 FORMAT (1H0,30X,4HO/F=F9.6,15H, PERCENT FUEL=F8.4,20H, EQUIVALENCE
     1 RATIO=F7.4,10H, DENSITY=F7.4)
      DO 60 I=1,13
   60 ASOL(I)=EXIT
      IF(IPROB-2)550,550,551
  550 NANA=2
      GO TO 552
  551 NANA=1
  552 REWIND 3
      KANE = NANA
      DO 200 ME=1,KANE
      KTAPE=0

  300 READ TAPE 3, (ANS(I),I=1,454)
      KTAPE=KTAPE+1
      HAL=ANS(2)*14.696006
      HALL=ANS(19)
      IF(ME-1)202,201,202
  201 LEN=NOEQ
      GO TO 203
  202 LEN=NOFROZ
  203 IF(LEN-13)102,102,103
  102 KODE=0
      GO TO 106
  103 KONT=0
      KODE=13
  106 J=34
      DO 104 I=1,N
      DO 105 II=1,3
      KK=J+II
  105 TITLE(II,I)=ANS(KK)
  104 J=J+4
      MAY=1
 1000 WRITE OUTPUT TAPE 6,18
   18 FORMAT (1H1)
      CALL HEAD
      ASSIGN 90 TO JEAN
   92 WRITE OUTPUT TAPE 6,2,KASE,HAL,OOF
      GO TO JEAN,(90,91)
   90 IF(KD)93,94,93
   94 WRITE OUTPUT TAPE 6,3
      GO TO 97
   93 WRITE OUTPUT TAPE 6,4
   97 IF(NF)351,350,351
  351 DO 100 I=1,NF
      II=I
      MM=15
      CALL SPEC
      IF(KD)401,400,401
  400 WRITE OUTPUT TAPE 6,5,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
      GO TO 100
  401 WRITE OUTPUT TAPE 6,6,A(I,34),A(I,32),A(I,42),A(I,44),A(I,36)
  100 CONTINUE
  350 IF(NO)353,352,353
  353 DO 101 I=1,NO
      II=I
      MM=0
      CALL SPEC
      IF(KD)411,410,411
  410 WRITE OUTPUT TAPE 6,5,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
      GO TO 101
  411 WRITE OUTPUT TAPE 6,6,A(I,33),A(I,31),A(I,41),A(I,43),A(I,35)
  101 CONTINUE
  352 CONTINUE
      WRITE OUTPUT TAPE 6,7,OOF,PERCF,EQUIV,HALL
      IF(KODE) 51,50,51
   50 IN=LEN
      GO TO 56
   51 IF(KONT) 53,52,53
   52 IN=KODE
      KONT=1
      GO TO 56
   53 IN=LEN -13
```

```
      KODE=0
   56 CALL READ
      IF(IPROB-2)600,600,601
  601 WRITE OUTPUT TAPE 6,602
  602 FORMAT (37H0EQUILIBRIUM THERMODYNAMIC PROPERTIES)
      CALL PERPAR
      GO TO 206
  600 WRITE OUTPUT TAPE 6,8
    8 FORMAT (11H0PARAMETERS)
      IF(MAY-1)64,63,64
   63 KK=IN-2
      WRITE OUTPUT TAPE 6,61,(ASOL(I),I=1, KK)
   61 FORMAT (1H0,16X,7HCHAMBER,4X,7HTHROAT ,10(3X,A6),3X,A4)
      GO TO 65
   64 WRITE OUTPUT TAPE 6,66,(ASOL(I),I=1,IN)
   66 FORMAT (1H0,15X,13(3X,A6))
   65 CONTINUE
      CALL PERPAR
      IF(ME-1)206,205,206
  205 WRITE OUTPUT TAPE 6,99
   99 FORMAT(1H )
      WRITE OUTPUT TAPE 6,9
    9 FORMAT (12H0DERIVATIVES)
      IF(MAY-1) 503,502,503
  503 CALL PERDER
      GO TO 504
  502 CALL PERDEY
  504 CONTINUE
  206 WRITE OUTPUT TAPE 6,99
      WRITE OUTPUT TAPE 6,10
   10 FORMAT (15H0MOLE FRACTIONS//)
      CALL COMP
  207 WRITE OUTPUT TAPE 6,16
   16 FORMAT (1H0,30X,16HINPUT, G-ATOMS/G//)
      IF(NE-8)80,80,81
   80 KK=1
      KKK=NE
      LOOP=1
      GO TO 82
   81 KK=1
      KKK=8
      LOOP=2
   82 DO 85 J=1,LOOP
      WRITE OUTPUT TAPE 6,11,(ELMT(I),I=KK,KKK)
   11 FORMAT (11X,8(6X,A2,7X))
      WRITE OUTPUT TAPE 6,12,(BOF (I),I=KK,KKK)
   12 FORMAT (5H FUEL,6X,8E15.7)
      WRITE OUTPUT TAPE 6,13,(BOX (I),I=KK,KKK)
   13 FORMAT (8H OXIDANT,3X,8E15.7)
      WRITE OUTPUT TAPE 6,14,(BO  (I),I=KK,KKK)
   14 FORMAT (11H PROPELLANT,8E15.7)
      IF (LOOP-1) 86,85,86
   86 KK=9
      KKK=NE
      WRITE OUTPUT TAPE 6,15
   15 FORMAT(1H0)
   85 CONTINUE
      ASSIGN 91 TO JEAN
      GO TO 92
   91 WRITE OUTPUT TAPE 6,119

  119 FORMAT (6H0NOTE.,2X,71HWEIGHT FRACTION OF FUEL IN TOTAL FUELS AND
     1OF OXIDANT IN TOTAL OXIDANTS)
      IF(KODE)96,95,96
   96 MAY=MAY+1
      GO TO 1000
   95 IF(NANA-1)208,200,208
  208 NANA=0
  200 CONTINUE
      RETURN
      END


      SUBROUTINE HEAD
C
C     OUTPUTS PROPER HEADING ACCORDING TO PROBLEM NUMBER
C
C
      COMMON C
      EQUIVALENCE (IPROB, C(2316)), (ME, C(1769))
  100 FORMAT (     25X,80HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB
     2RIUM COMPOSITION DURING EXPANSION)
  200 FORMAT (     25X,75HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
     2COMPOSITION DURING EXPANSION)
  300 FORMAT (     25X,80HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIB
     2RIUM COMPOSITION DURING EXPANSION/44X,28HFROM AN ASSIGNED TEMPERAT
     3URE)
  400 FORMAT (     25X,75HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN
     2COMPOSITION DURING EXPANSION/44X,28HFROM AN ASSIGNED TEMPERATURE)
  500 FORMAT (     25X,74HTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE
     2D PRESSURE AND TEMPERATURES)
  600 FORMAT (     25X,74HTHEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNE
     2D TEMPERATURE AND PRESSURES)
      IF(IPROB-2)1,2,10
   10 IF(IPROB-4)3,4,4
    1 IF(ME-1)12,11,12
   11 WRITE OUTPUT TAPE 6,100
      RETURN
   12 WRITE OUTPUT TAPE 6,200
      RETURN
    2 IF(ME-1)14,13,14
   13 WRITE OUTPUT TAPE 6,300
      RETURN
   14 WRITE OUTPUT TAPE 6,400
      RETURN
    3 WRITE OUTPUT TAPE 6,500
      RETURN
    4 WRITE OUTPUT TAPE 6,600
      RETURN
      END


      SUBROUTINE PERDER
C
C     OUTPUTS PERFORMANCE DERIVATIVES
C
C
      COMMON C
      EQUIVALENCE (IN, C(8046))
      EQUIVALENCE (PER(1), C(10498)),  (PER(169), C(10606))
      DIMENSION PER(13,13)
```

```
  1 FORMAT (15HO(DLI/DLPC)PC/P13F9.5)
  2 FORMAT (15H (DLT/DLPC)PC/P13F9.5)
  3 FORMAT (16H (DLAR/DLPC)PC/PF8.5,12F9.5)
  4 FORMAT (16H (DLCS/DLPC)PC/PF8.5,12F9.5)
  5 FORMAT (15HO(DLI/DHC)PC/P*13F9.5)
  6 FORMAT (15H (DLT/DHC)PC/P*13F9.5)
  7 FORMAT (16H (DLAR/DHC)PC/P*F8.5,12F9.5)
  8 FORMAT (16H (DLCS/DHC)PC/P*F8.5,12F9.5)
  9 FORMAT (16H *(HC IN KCAL/G))
 10 FORMAT (13HO(DLI/DLPCP)S,2X,13F9.5)
 11 FORMAT (13H (DLT/DLPCP)S,2X,13F9.5)
 12 FORMAT (15H (DLAR/DLPCP)S 13F9.5)
    WRITE OUTPUT TAPE 6,1,(PER(I,2),I=1,IN)
    WRITE OUTPUT TAPE 6,2,(PER(I,1),I=1,IN)
    WRITE OUTPUT TAPE 6,3,(PER(I,3),I=1,IN)
    WRITE OUTPUT TAPE 6,4,(PER(I,5),I=1,IN)
    WRITE OUTPUT TAPE 6,5,(PER(I,7),I=1,IN)
    WRITE OUTPUT TAPE 6,6,(PER(I,6),I=1,IN)
    WRITE OUTPUT TAPE 6,7,(PER(I,8),I=1,IN)
    WRITE OUTPUT TAPE 6,8,(PER(I,10),I=1,IN)
    WRITE OUTPUT TAPE 6,9
    WRITE OUTPUT TAPE 6,10,(PER(I,12),I=1,IN)
    WRITE OUTPUT TAPE 6,11,(PER(I,11),I=1,IN)
    WRITE OUTPUT TAPE 6,12,(PER(I,13),I=1,IN)
    RETURN
    END


    SUBROUTINE PERDEY
C
C   OUTPUTS PERFORMANCE DERIVATIVES
C
C
    COMMON C
    EQUIVALENCE (IN, C(8046))
    EQUIVALENCE (PER(1), C(10438)),  (PER(169), C(10606))
    DIMENSION PER(13,13)
  1 FORMAT (15HO(DLI/DLPC)PC/P,9X,12F9.5)
  2 FORMAT (15H (DLT/DLPC)PC/P13F9.5)
  3 FORMAT (16H (DLAR/DLPC)PC/P,8X,12F9.5)
  4 FORMAT (16H (DLCS/DLPC)PC/P,8X,12F9.5)
  5 FORMAT (15HO(DLI/DHC)PC/P*,9X,12F9.5)
  6 FORMAT (15H (DLT/DHC)PC/P*13F9.5)
  7 FORMAT (16H (DLAR/DHC)PC/P*,8X,12F9.5)
  8 FORMAT (16H (DLCS/DHC)PC/P*,8X,12F9.5)
  9 FORMAT (16H *(HC IN KCAL/G))
 10 FORMAT (13HO(DLI/DLPCP)S,11X,12F9.5)
 11 FORMAT (13H (DLT/DLPCP)S,2X,13F9.5)
 12 FORMAT (15H (DLAR/DLPCP)S,9X,12F9.5)
    WRITE OUTPUT TAPE 6,1,(PER(I,2),I=2,IN)
    WRITE OUTPUT TAPE 6,2,(PER(I,1),I=1,IN)
    WRITE OUTPUT TAPE 6,3,(PER(I,3),I=2,IN)
    WRITE OUTPUT TAPE 6,4,(PER(I,5),I=2,IN)
    WRITE OUTPUT TAPE 6,5,(PER(I,7),I=2,IN)
    WRITE OUTPUT TAPE 6,6,(PER(I,6),I=1,IN)
    WRITE OUTPUT TAPE 6,7,(PER(I,8),I=2,IN)
    WRITE OUTPUT TAPE 6,8,(PER(I,10),I=2,IN)
    WRITE OUTPUT TAPE 6,9
    WRITE OUTPUT TAPE 6,10,(PER(I,12),I=2,IN)
    WRITE OUTPUT TAPE 6,11,(PER(I,11),I=1,IN)

    WRITE OUTPUT TAPE 6,12,(PER(I,13),I=2,IN)
    RETURN
    END


    SUBROUTINE READ
C
C   SORTS WHAT IS ON TAPE 3
C
C
    COMMON C
    EQUIVALENCE   (ANS(1),  C(421)),  (ANS(454),    C(874))
    EQUIVALENCE (LEN, C(1766)), (MAY, C(1767))
    EQUIVALENCE (LOOP, C(1770)), (KTAPE, C(8045))
    EQUIVALENCE (IN, C(8046))
    EQUIVALENCE  (NN,   C(2329))
    EQUIVALENCE (PAR(1), C(8370)), (PAR(208), C(8577))
    EQUIVALENCE (AMOL(1),  C(9268)), (AMOL(1170), C(10437))
    EQUIVALENCE (DER(1), C(10438)),  (DER(169), C(10606))
    DIMENSION PAR(13,16),DER(13,13),              ANS(454)
    DIMENSION AMOL(13,90)
    DO 1 I=1,IN
    DO 2 J=1,16
  2 PAR(I,J)=ANS(J)
    N=1
    DO 3 J=20,32
    DER(I,N)=ANS(J)
  3 N=N+1
    N=1
    J=38
    DO 4 JJ=1,NN
    AMOL(I,N)=ANS(J)
    J=J+4
  4 N=N+1
    IF(KTAPE-LEN)100,1,100
100 RE\D TAPE 3,(ANS(K),K=1,454)
    KTAPE=KTAPE+1
  1 CONTINUE
    RETURN
    END


    SUBROUTINE PERPAR
C
C   OUTPUTS PERFORMANCE PARAMETERS
C
C
    COMMON C
    EQUIVALENCE (KODE, C(1768))
    EQUIVALENCE (IN, C(8046)),  (MAY, C(1767))
    EQUIVALENCE (PAR(1), C(8370)), (PAR(208), C(8577))
    DIMENSION PAR(13,16),NN(13)
 10 FORMAT (5H PC/P,10X)
 11 FORMAT (8H P, ATM ,7X)
 12 FORMAT (9H T, DEG K,6X,13I9)
 13 FORMAT (9H H, CAL/G,6X,13F9.1)
 14 FORMAT (15H S, CAL/(G)(K) 13F9.4)
 15 FORMAT (10HOM, MOL WT,5X,13F9.3)
 16 FORMAT (11H (DLM/DLP)T,4X,13F9.5)
 17 FORMAT (11H (DLM/DLT)P,4X,13F9.4)
```

```
   18 FORMAT (15H CP, CAL/(G)(K)13F9.4)
   19 FORMAT (6H GAMMA,9X,13F9.4)
   20 FORMAT (12H MACH NUMBEH,3X,13F9.3)
   21 FORMAT (15HOCSTAR, FT/SEC 13I9)
   22 FORMAT (3H CF,12X,13F9.3)
   23 FORMAT (6H AE/AT,9X,13F9.3)
   24 FORMAT (15H IVAC,LB-SEC/LB13F9.1)
   25 FORMAT (15H I, LB-SEC/LB  13F9.1)
      IF(KODE-1)2,1,2
    1 WRITE OUTPUT TAPE 6,111
  111 FORMAT (8HOP, ATM ,7X)
      GO TO 3
    2 WRITE OUTPUT TAPE 6,10
      CALL VAR(1)
      WRITE OUTPUT TAPE 6,11
    3 CALL VAR(2)
      DO 60 I=1,IN
   60 NN(I)=PAR(I,3)+.5
      WRITE OUTPUT TAPE 6,12,(NN(I),I=1,IN)
      WRITE OUTPUT TAPE 6,13,(PAR(I,4),I=1,IN)
      WRITE OUTPUT TAPE 6,14,(PAR(I,5),I=1,IN)
      WRITE OUTPUT TAPE 6,15,(PAR(I,6),I=1,IN)
      IF(KODE)6,5,6
    6 WRITE OUTPUT TAPE 6,16,(PAR(I,8),I=1,IN)
      WRITE OUTPUT TAPE 6,17,(PAR(I,9),I=1,IN)
    5 WRITE OUTPUT TAPE 6,18,(PAR(I,7),I=1,IN)
      WRITE OUTPUT TAPE 6,19,(PAR(I,10),I=1,IN)
      IF(KODE-1)41,40,41
   40 RETURN
   41 WRITE OUTPUT TAPE 6,20,(PAR(I,12),I=1,IN)
      DO 61 I=1,IN
   61 NN(I)=PAR(I,15)+.5
      IF (MAY-1) 51,50,51
   50 WRITE OUTPUT TAPE 6,31,(NN(I),I=2,IN)
      WRITE OUTPUT TAPE 6,32,(PAR(I,16),I=2,IN)
      WRITE OUTPUT TAPE 6,33
      CALL VAR(11)
      WRITE OUTPUT TAPE 6,34,(PAR(I,14),I=2,IN)
      WRITE OUTPUT TAPE 6,35,(PAR(I,13),I=2,IN)
   31 FORMAT (15HOCSTAR, FT/SEC ,9X,12I9)
   32 FORMAT (3H CF,21X,12F9.3)
   33 FORMAT (6H AE/AT,18X,12F9.3)
   34 FORMAT (15H IVAC,LB-SEC/LB,9X,12F9.1)
   35 FORMAT (15H I, LB-SEC/LB ,9X,12F9.1)
      RETURN
   51 WRITE OUTPUT TAPE 6,21,(NN(I),I=1,IN)
      WRITE OUTPUT TAPE 6,22,(PAR(I,16),I=1,IN)
      WRITE OUTPUT TAPE 6,23
      CALL VAR(11)
      WRITE OUTPUT TAPE 6,24,(PAR(I,14),I=1,IN)
      WRITE OUTPUT TAPE 6,25,(PAR(I,13),I=1,IN)
      RETURN
      END


      SUBROUTINE VAR(INDEX)
C
C     SPECIAL FORMAT FOR PC/P,P, AND AE/AT
C
C


      COMMON C
      EQUIVALENCE (IN, C(8046)), (MAY, C(1767))
      EQUIVALENCE (PAR(1), C(8370)), (PAR(208), C(8577))
      DIMENSION FMT(3),PAR(13,16),TEM(4),AM(4),TEMM(13)
B     ZERO=113300346060
B     ONE=113301346060
B     TWO=113302346060
B     THR=113303346060
B     FR=113304346060
B     TEMM(1)=600104677326
B     TEMM(2)=600203677326
B     TEMM(3)=600302677326
B     TEMM(4)=600401677326
B     TEMM(5)=600500677326
B     TEMM(6)=600511677326
B     TEMM(7)=600610677326
B     TEMM(8)=600707677326
B     TEMM(9)=601006677326
B     TEMM(10)=601105677326
B     TEMM(11)=010004677326
B     TE'M(12)=010103677326
B     TEMM(13)=010202677326
B     FMT(1)=740130207360
      IF(INDEX-2) 1,2,3
    1 TEM(1)=1.0E04
      TEM(2)=1.0E05
      TEM(3)=1.0E06
      AM(1)=THR
      AM(2)=TWO
      AM(3)=ONE
      AM(4)=ZERO
      GO TO 4
    2 TEM(1)=1.0
      TEM(2)=10.0
      TEM(3)=100.0
      AM(1)=FR
      AM(2)=THR
      AM(3)=TWO
      AM(4)=ONE
      GO TO 4
    3 TEM(1)=10.0
      TEM(2)=100.0
      TEM(3)=1000.0
      AM(1)=THR
      AM(2)=TWO
      AM(3)=ONE
      AM(4)=ZERO
    4 DO 5 I=1,IN
      IF (I-1) 53,50,53
   50 IF (MAY-1) 53,52,53
   52 IF(INDEX-11) 53,5,53
   53 CONTINUE
      FMT(2)=TEMM(I)
      DO 6 J=1,3
      IF(PAR(I,INDEX)-TEM(J))10,6,6
   10 FMT(3)=AM(J)
   11 WRITE OUTPUT TAPE 6,FMT,PAR(I,INDEX)
      GO TO 5
    6 CONTINUÉ
      FMT(3)=AM(4)

      WRITE OUTPUT TAPE 6,FMT,PAR(I,INDEX)
    5 CONTINUE
      RETURN
```

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TABLE I. - ITERATION EQUATIONS TO DETERMINE EQUILIBRIUM COMPOSITIONS FOR EITHER ASSIGNED PRESSURE AND TEMPERATURE, ASSIGNED PRESSURE AND ENTHALPY, OR ASSIGNED PRESSURE AND ENTROPY

$\Delta \ln u_1$	$\Delta \ln u_2$	$\Delta \ln u_3$	. . . .	Δn_{n-1}	Δn_n	$-\Delta \ln A$	$\Delta \ln T$ (*)	Constant
r_{11}	r_{12}	r_{13}	. . . .	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^{n} a_{1,k} n_k$	$\sum_{k=1}^{m} a_{1,k} \mathscr{H}_k n_k$	$A\,\Delta b_1 + \sum_{k=1}^{m} a_{1,k} n_k \mathscr{F}_k$
r_{21}	r_{22}	r_{23}	. . . .	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^{n} a_{2,k} n_k$	$\sum_{k=1}^{m} a_{2,k} \mathscr{H}_k n_k$	$A\,\Delta b_2 + \sum_{k=1}^{m} a_{2,k} n_k \mathscr{F}_k$
r_{31}	r_{32}	r_{33}	. . . .	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^{n} a_{3,k} n_k$	$\sum_{k=1}^{m} a_{3,k} \mathscr{H}_k n_k$	$A\,\Delta b_3 + \sum_{k=1}^{m} a_{3,k} n_k \mathscr{F}_k$
. . .	. . .	. . .	. . . .	. . .	. . .	. . .	. . .	. . .
. . .	. . .	. . .	. . . .	. . .	. . .	. . .	. . .	. . .
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	. . . .	0	0	0	$\mathscr{H}_{n-1}$	$\mathscr{F}_{n-1}$
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	. . . .	0	0	0	$\mathscr{H}_n$	$\mathscr{F}_n$
$\sum_{k=1}^{m} a_{1,k} n_k$	$\sum_{k=1}^{m} a_{2,k} n_k$	$\sum_{k=1}^{m} a_{3,k} n_k$	. . . .	0	0	0	$\sum_{k=1}^{m} \mathscr{H}_k n_k$	$\sum_{k=1}^{m} \mathscr{F}_k n_k + \Delta P$
$\sum_{k=1}^{m} a_{1,k} \mathscr{H}_k n_k$	$\sum_{k=1}^{m} a_{2,k} \mathscr{H}_k n_k$	$\sum_{k=1}^{m} a_{3,k} \mathscr{H}_k n_k$	. . . .	$\mathscr{H}_{n-1}$	$\mathscr{H}_n$	$\sum_{k=1}^{n} \mathscr{H}_k n_k$	$\sum_{k=1}^{n} \mathscr{C}_k n_k + \sum_{k=1}^{m} \mathscr{H}_k \mathscr{H}_k n_k$	$A\,\Delta h + \sum_{k=1}^{m} \mathscr{H}_k n_k \mathscr{F}_k$
$\sum_{k=1}^{m} a_{1,k} \mathscr{S}_k n_k$	$\sum_{k=1}^{m} a_{2,k} \mathscr{S}_k n_k$	$\sum_{k=1}^{m} a_{3,k} \mathscr{S}_k n_k$	. . . .	$\mathscr{S}_{n-1}$	$\mathscr{S}_n$	$\sum_{k=1}^{n} \mathscr{S}_k n_k$	$\sum_{k=1}^{n} \mathscr{C}_k n_k + \sum_{k=1}^{m} \mathscr{S}_k \mathscr{H}_k n_k$	$A\,\Delta \mathscr{S} + \Delta P + \sum_{k=1}^{m} \mathscr{S}_k n_k \mathscr{F}_k$

Iteration for assigned pressure and temperature (rows from r_{11} through the row $\sum_{k=1}^{m} a_{1,k} n_k$)

Iteration for assigned pressure and enthalpy (rows from r_{11} through the row $\sum_{k=1}^{m} a_{1,k} \mathscr{H}_k n_k$)

Iteration for assigned pressure and entropy (rows from r_{11} through the row $\sum_{k=1}^{m} a_{1,k} n_k$, and the row $\sum_{k=1}^{m} a_{1,k} \mathscr{S}_k n_k$)

* This column not used for assigned pressure and temperature.

TABLE II. - EQUATIONS FOR EVALUATING DERIVATIVES WITH RESPECT TO LOGARITHM OF TEMPERATURE AT CONSTANT PRESSURE

$\left(\frac{\partial \ln u_1}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_2}{\partial \ln T}\right)_P$	$\left(\frac{\partial \ln u_3}{\partial \ln T}\right)_P$	. . .	. . .	$\left(\frac{\partial n_{n-1}}{\partial \ln T}\right)_P$	$\left(\frac{\partial n_n}{\partial \ln T}\right)_P$	$-\left(\frac{\partial \ln A}{\partial \ln T}\right)_P$	Constant
r_{11}	r_{12}	r_{13}	. . .	. . .	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^{n} a_{1,k}n_k$	$-\sum_{k=1}^{m} a_{1,k}\mathcal{H}_k n_k$
r_{21}	r_{22}	r_{23}	. . .	. . .	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^{n} a_{2,k}n_k$	$-\sum_{k=1}^{m} a_{2,k}\mathcal{H}_k n_k$
r_{31}	r_{32}	r_{33}	. . .	. . .	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^{n} a_{3,k}n_k$	$-\sum_{k=1}^{m} a_{3,k}\mathcal{H}_k n_k$
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	. . .	. . .	0	0	0	$-\mathcal{H}_{n-1}$
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	. . .	. . .	0	0	0	$-\mathcal{H}_n$
$\sum_{k=1}^{m} a_{1,k}n_k$	$\sum_{k=1}^{m} a_{2,k}n_k$	$\sum_{k=1}^{m} a_{3,k}n_k$	. . .	. . .	0	0	0	$-\sum_{k=1}^{m} \mathcal{H}_k n_k$

TABLE III. - EQUATIONS FOR EVALUATING DERIVATIVES WITH RESPECT TO

LOGARITHM OF A AT CONSTANT TEMPERATURE

$\left(\frac{\partial \ln u_1}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_2}{\partial \ln A}\right)_T$	$\left(\frac{\partial \ln u_3}{\partial \ln A}\right)_T$	. . .	. . .	$\left(\frac{\partial n_{n-1}}{\partial \ln A}\right)_T$	$\left(\frac{\partial n_n}{\partial \ln A}\right)_T$	Constant
r_{11}	r_{12}	r_{13}	. . .	. . .	$a_{1,n-1}$	$a_{1,n}$	$\sum_{k=1}^{n} a_{1,k}n_k$
r_{21}	r_{22}	r_{23}	. . .	. . .	$a_{2,n-1}$	$a_{2,n}$	$\sum_{k=1}^{n} a_{2,k}n_k$
r_{31}	r_{32}	r_{33}	. . .	. . .	$a_{3,n-1}$	$a_{3,n}$	$\sum_{k=1}^{n} a_{3,k}n_k$
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .
. . .	. . .	. . .	. . .	. . .	. . .	. . .	. . .
$a_{1,n-1}$	$a_{2,n-1}$	$a_{3,n-1}$	. . .	. . .	0	0	0
$a_{1,n}$	$a_{2,n}$	$a_{3,n}$	. . .	. . .	0	0	0

TABLE IV. - FIRST DERIVATIVES OF SOME THERMODYNAMIC PROPERTIES AND ROCKET PERFORMANCE PARAMETERS

A	$\left(\frac{\partial \ln A}{\partial \ln P_c}\right)_{P_c/P,h_c}$	$\left(\frac{\partial \ln A}{\partial \ln h_c}\right)_{P_c/P,P_c}$	$\left(\frac{\partial \ln A}{\partial \ln P_c}\right)_{h_c,P}$	$\left(\frac{\partial \ln A}{\partial \ln \frac{P_c}{P}}\right)_{P_c,h_c} = \left(\frac{\partial \ln A}{\partial \ln \frac{P_c}{P}}\right)_s = -\left(\frac{\partial \ln A}{\partial \ln P}\right)_s$
T	$\frac{R}{c_pM}\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right] - \frac{R}{c_pM_c}$	$\frac{h_c}{c_pT_c}$	$-\frac{R}{c_pM_c}$	$\frac{R}{c_pM}\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right]$
h	$\frac{RT}{h}\left(\frac{1}{M} - \frac{1}{M_c}\right)$	$\frac{h_cT}{hT_c}$	$-\frac{RT}{hM_c}$	$-\frac{RT}{hM}$
ρ	$\frac{R}{c_pM_c}\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right] + \frac{1}{\gamma}$	$-\frac{h_c}{c_pT_c}\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]$	$\frac{R}{M_cc_p}\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]$	$-\left(\frac{\partial \ln \rho}{\partial \ln P}\right)_s = -\frac{1}{\gamma}$
M	$\left(\frac{\partial \ln M}{\partial \ln T}\right)_P\left(\frac{\partial \ln T}{\partial \ln P_c}\right)_{P_c/P,h_c} + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T$	$\left(\frac{\partial \ln M}{\partial \ln T}\right)_P\left(\frac{\partial \ln T}{\partial \ln h_c}\right)_{P_c/P,P_c}$	$\left(\frac{\partial \ln M}{\partial \ln T}\right)_P\left(\frac{\partial \ln T}{\partial \ln P_c}\right)_{h_c,P}$	$\left(\frac{\partial \ln M}{\partial \ln T}\right)_P\left(\frac{\partial \ln T}{\partial \ln \frac{P_c}{P}}\right)_s - \left(\frac{\partial \ln M}{\partial \ln P}\right)_T$
I	$\frac{RT}{2(h_c - h)}\left(\frac{1}{M_c} - \frac{1}{M}\right)$	$\frac{h_c}{2T_c}\left(\frac{T_c - T}{h_c - h}\right)$	$\frac{RT}{2(h_c - h)M_c}$	$\frac{RT}{2(h_c - h)M}$
$\frac{A}{w}$	$-\left(\frac{\partial \ln I}{\partial \ln P_c}\right)_{P_c/P,h_c} - \left(\frac{\partial \ln \rho}{\partial \ln P_c}\right)_{P_c/P,h_c}$	$-\left(\frac{\partial \ln I}{\partial \ln h_c}\right)_{P_c/P,P_c} - \left(\frac{\partial \ln \rho}{\partial \ln h_c}\right)_{P_c/P,P_c}$	$-\left(\frac{\partial \ln I}{\partial \ln P_c}\right)_{h_c,P} - \left(\frac{\partial \ln \rho}{\partial \ln P_c}\right)_{h_c,P}$	$-\left(\frac{\partial \ln I}{\partial \ln \frac{P_c}{P}}\right)_s - \left(\frac{\partial \ln \rho}{\partial \ln \frac{P_c}{P}}\right)_s$
ϵ	$\left(\frac{\partial \ln \frac{A}{w}}{\partial \ln P_c}\right)_{P_c/P,h_c} - \left[\frac{\partial \ln\left(\frac{A}{w}\right)_t}{\partial \ln P_c}\right]_{P_c/P,h_c}$	$\left(\frac{\partial \ln \frac{A}{w}}{\partial \ln h_c}\right)_{P_c/P,P_c} - \left[\frac{\partial \ln\left(\frac{A}{w}\right)_t}{\partial \ln h_c}\right]_{P_c/P,P_c}$	$\left(\frac{\partial \ln \frac{A}{w}}{\partial \ln P_c}\right)_{h_c,P} - \left[\frac{\partial \ln\left(\frac{A}{w}\right)_t}{\partial \ln P_c}\right]_{h_c,P}$	$\left(\frac{\partial \ln \frac{A}{w}}{\partial \ln \frac{P_c}{P}}\right)_s$
c^*	$1 + \left[\frac{\partial \ln\left(\frac{A}{w}\right)_t}{\partial \ln P_c}\right]_{P_c/P,h_c}$	$\left[\frac{\partial \ln\left(\frac{A}{w}\right)_t}{\partial \ln h_c}\right]_{P_c/P,P_c}$	$1 + \left[\frac{\partial \ln\left(\frac{A}{w}\right)_t}{\partial \ln P_c}\right]_{h_c,P}$	0
I_{vac}	$\frac{1}{I_{vac}}\left\{I\left(\frac{\partial \ln I}{\partial \ln P_c}\right)_{P_c/P,h_c} + \frac{PA}{w}\left[1 + \left(\frac{\partial \ln \frac{A}{w}}{\partial \ln P_c}\right)_{P_c/P,h_c}\right]\right\}$	$\frac{1}{I_{vac}}\left\{I\left(\frac{\partial \ln I}{\partial \ln h_c}\right)_{P_c/P,P_c} + \frac{PA}{w}\left[1 + \left(\frac{\partial \ln \frac{A}{w}}{\partial \ln h_c}\right)_{P_c/P,P_c}\right]\right\}$	$\frac{1}{I_{vac}}\left\{I\left(\frac{\partial \ln I}{\partial \ln P_c}\right)_{h_c,P} + \frac{PA}{w}\left[1 + \left(\frac{\partial \ln \frac{A}{w}}{\partial \ln P_c}\right)_{h_c,P}\right]\right\}$	$\frac{1}{I_{vac}}\left\{I\left(\frac{\partial \ln I}{\partial \ln \frac{P_c}{P}}\right)_s + \frac{PA}{w}\left[1 + \left(\frac{\partial \ln \frac{A}{w}}{\partial \ln \frac{P_c}{P}}\right)_s\right]\right\}$
C_F	$\left(\frac{\partial \ln I}{\partial \ln P_c}\right)_{P_c/P,h_c} - \left(\frac{\partial \ln c^*}{\partial \ln P_c}\right)_{P_c/P,h_c}$	$\left(\frac{\partial \ln I}{\partial \ln h_c}\right)_{P_c/P,P_c} - \left(\frac{\partial \ln c^*}{\partial \ln h_c}\right)_{P_c/P,P_c}$	$\left(\frac{\partial \ln I}{\partial \ln P_c}\right)_{h_c,P} - \left(\frac{\partial \ln c^*}{\partial \ln P_c}\right)_{h_c,P}$	$\left(\frac{\partial \ln I}{\partial \ln \frac{P_c}{P}}\right)_s$

TABLE V. - NEWTON-RAPHSON ITERATION EQUATIONS FOR

CALCULATING CHAPMAN-JOUGUET DETONATIONS

$$\left\{\frac{P_1}{P} - \gamma\left(\frac{\rho}{\rho_1}\right)\left[1 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right]\right\}\Delta \ln \frac{P}{P_1} + \left\{\gamma\left(\frac{\rho}{\rho_1}\right)\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]\right\}\Delta \ln \frac{T}{T_1} = \frac{P_1}{P} + \gamma\left(\frac{\rho}{\rho_1} - 1\right) - 1$$

$$\left(\frac{\gamma}{2}\left\{\left(\frac{\rho}{\rho_1}\right)^2\left[2 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right\} - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right)\Delta \ln \frac{P}{P_1} + \left\{\frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2 + 1\right]\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right] - \frac{Mc_p}{R}\right\}\Delta \ln \frac{T}{T_1} = \frac{M}{RT}(h - h_1) - \frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2 - 1\right]$$

TABLE VI. - SIMULTANEOUS EQUATIONS FOR OBTAINING PARTIAL DERIVATIVES OF DETONATION PRESSURE, TEMPERATURE, AND VELOCITY

$$\left\{\frac{P_1}{P} - \gamma\left(\frac{\rho}{\rho_1}\right)\left[1 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right]\right\} X_1 + \left\{\gamma\left(\frac{\rho}{\rho_1}\right)\left[1 - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right]\right\} X_2 = C_1$$

$$\left\{\frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2\left[2 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right] - \left(\frac{\partial \ln M}{\partial \ln T}\right)_P\right\} X_1 + \left\{\frac{\gamma}{2}\left[\left(\frac{\rho}{\rho_1}\right)^2 + 1\right]\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right] - \frac{Mc_p}{R}\right\} X_2 = C_2$$

Variable	X_1	X_2	C_1	C_2	Detonation velocity derivative
T_1	$\left(\frac{\partial \ln P}{\partial \ln T_1}\right)_{P_1}$	$\left(\frac{\partial \ln T}{\partial \ln T_1}\right)_{P_1}$	$\gamma\left(\frac{\rho}{\rho_1}\right)$	$-\gamma\left(\frac{\rho}{\rho_1}\right)^2 - \frac{M}{R}(c_p)_f \frac{T_1}{T}$	* $\left(\frac{\partial u_D}{\partial \ln T_1}\right)_{P_1} = u_D[AX_1 + BX_2 + 1]$
P_1	$\left(\frac{\partial \ln P}{\partial \ln P_1}\right)_{T_1,h_1}$	$\left(\frac{\partial \ln T}{\partial \ln P_1}\right)_{T_1,h_1}$	$\frac{P_1}{P} - \gamma\left(\frac{\rho}{\rho_1}\right)$	$\gamma\left(\frac{\rho}{\rho_1}\right)^2$	$\left(\frac{\partial u_D}{\partial \ln P_1}\right)_{T_1,h_1} = u_D[AX_1 + BX_2 - 1]$
h_1	$\left(\frac{\partial \ln P}{\partial h_1}\right)_{P_1,T_1}$	$\left(\frac{\partial \ln T}{\partial h_1}\right)_{P_1,T_1}$	0	$-\frac{M}{RT}$	$\left(\frac{\partial u_D}{\partial h_1}\right)_{P_1,T_1} = u_D[AX_1 + BX_2]$

* $A = \frac{1}{2}\left[2 + \left(\frac{\partial \ln M}{\partial \ln P}\right)_T\right]$ and $B = \frac{1}{2}\left[\left(\frac{\partial \ln M}{\partial \ln T}\right)_P - 1\right]$.

TABLE VII. - SIMULTANEOUS LEAST SQUARES FITTING OF HEAT CAPACITY, ENTHALPY, AND ENTROPY

Heat capacity: $\frac{C_p^o}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4.$

Enthalpy: $\frac{H_T^o - H_0^o}{RT} = a_1 + a_2\frac{T}{2} + a_3\frac{T^2}{3} + a_4\frac{T^3}{4} + a_5\frac{T^4}{5} + \frac{a_6 - (H_0^o/R)}{T}.$

Entropy: $\frac{S_T^o}{R} = a_1 \ln T + a_2T + a_3\frac{T^2}{2} + a_4\frac{T^3}{3} + a_5\frac{T^4}{4} + a_7.$

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

*p is the number of temperature points used to fit data.

TABLE VIII. - PROGRAM INPUT

Card type	Card name	Optional card?	Number of cards	Card format
1	Reactant	No	1-30 (1-15 oxidants) (1-15 fuels)	(5(A2,F7.5),F8.5,F9.5,A1,F8.5,A1,I1,F8.5)
	Blank	No	1	
2	Omit-Insert	Yes	Any	(4(2A6,3X))
	Blank	No	1	
3	Problem (H,S;T,S;T,P;P,T; or DETN), case	No	1	(A5,I5)
[a] 4	Schedule (of P_c/P, or P, or T)	No	1-5	(5F10.2)
	Blank[a]	No	1	
5	Mixture ($\mathcal{R}$, O/F, %F, P, T, code, debug)	No	Any	(5F10.2,I5,16X,I1)
	Blank[b]	No	1-3	

[a] For DETN problems, the schedule cards and the blank card that follows them must be omitted.

[b] There may be one, two, or three blank cards.
(1) One blank card: Program returns to read another sequence of cards starting with type 3.
(2) Two blank cards: Program returns to read another sequence of cards starting with type 1.
(3) Three blank cards: Program terminates.

TABLE IX. - EXAMPLES OF TYPICAL REACTANT CARDS

	Content				Reactant formula						Relative weights (a)	Enthalpy, cal/(g)(mole)	State	Temperature, ^{o}K	Fuel or oxidant	Density, g/cc, or heat capacity, cal/(g)(mole)(^{o}K)
Columns	1-2	3-9	10-11	12-18	19-20	21-27	28-29	30-36	37-38	39-45	46-53	54-62	63	64-71	72	73-80
	N	1.	H	4.	CL	1.	O	4.			72.06	-70730.	S	298.15	F	
	C	1.	H	1.86955	O	.03126	S	.00841			18.58	-2999.082	L	298.15	F	
	AL	1.									9.	0.	S	298.15	F	
	MG	1.	O	1.							.2	143700.	S	298.15	F	
	H	2.	O	1.							.16	-68317.4	L	298.15	F	
	H	2.									100.	0.	G	298.15	F	
	N	.780881	O	.209795	AR	.004662	C	.00015			100.	-7.202	G	298.15	O	
	H	2.									100.	0.	G	298.15	F	6.8922
	O	2.									100.	0.	G	298.15	O	7.0215

[a] Relative weight of fuel in total fuels or oxidant in total oxidants as designated in column 72.

TABLE X. - THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

CASE NO. 51 500.0 0.

	CHEMICAL FORMULA				WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 1.00000	H 4.00000	CL 1.00000	O 4.00000	0.72060	-70730.000	S	298.15	-0.
FUEL	H 1.86955	O 0.03126	C 1.00000	S 0.00841	0.18580	-2999.082	L	298.15	-0.
FUEL	AL 1.00000				0.09000	0.	S	298.15	-0.
FUEL	O 1.00000	MG 1.00000			0.00200	-143700.000	S	298.15	-0.
FUEL	H 2.00000	O 1.00000			0.00160	-68317.399	L	298.15	-0.

O/F= 0. , PERCENT FUEL=100.0000, EQUIVALENCE RATIO= 1.9480, DENSITY= 0.

PARAMETERS

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.777	2.500	2.750	3.000	3.250	3.500	4.000	10.000	34.023	100.000	1000.000	10000.00
P, ATM	34.02	19.15	13.61	12.37	11.34	10.47	9.721	8.506	3.402	1.000	0.3402	0.0340	0.0034
T, DEG K	2737	2492	2351	2317	2317	2317	2302	2248	1900	1503	1219	790	529
H, CAL/G	-485.0	-613.9	-684.7	-703.7	-721.0	-736.8	-751.5	-777.5	-939.7	-1117.0	-1241.9	-1436.0	-1563.1
S, CAL/(G)(K)	2.5264	2.5264	2.5265	2.5264	2.5265	2.5265	2.5265	2.5264	2.5264	2.5264	2.5264	2.5264	2.5264
M, MOL WT	23.126	23.192	23.217	23.221	23.220	23.218	23.220	23.227	23.251	23.256	23.256	23.256	23.422
(DLM/DLP)T	0.00294	0.00147	0.00092	0.	0.	0.	0.00085	0.00069	0.00013	0.00001	0.00000	-0.00000	0.01402
(DLM/DLT)P	-0.0586	-0.0310	-0.0200	0.	0.	0.	-0.0190	-0.0156	-0.0032	-0.0002	-0.0000	0.0000	-0.3080
CP, CAL/(G)(K)	0.5783	0.5265	0.5037	0.4606	0.4582	0.4560	0.4959	0.4881	0.4551	0.4441	0.4402	0.4699	0.9971
GAMMA	1.1956	1.2071	1.2134	1.2282	1.2297	1.2310	1.2171	1.2197	1.2329	1.2384	1.2409	1.2223	1.1515
MACH NUMBER	0.	1.000	1.279	1.340	1.391	1.436	1.491	1.579	2.132	2.819	3.422	4.803	6.458
CSTAR, FT/SEC		5015	5015	5015	5015	5015	5015	5015	5015	5015	5015	5015	5015
CF		0.679	0.846	0.885	0.919	0.950	0.977	1.024	1.276	1.504	1.646	1.846	1.965
AE/AT		1.000	1.065	1.103	1.159	1.215	1.264	1.346	2.278	5.200	11.33	65.47	409.2
IVAC,LB-SEC/LB		193.6	198.2	200.5	203.5	206.3	208.6	212.0	234.4	258.3	274.3	297.9	312.7
I, LB-SEC/LB ,		105.9	131.8	138.0	143.3	148.0	152.3	159.5	198.9	234.5	256.6	287.7	306.3

DERIVATIVES

(DLI/DLPC)PC/P		0.00237	0.00198	0.00187	0.00170	0.00157	0.00149	0.00143	0.00096	0.00057	0.00039	0.00020	0.00027
(DLT/DLPC)PC/P	0.00871	0.00459	0.00273	-0.00077	-0.00076	-0.00075	0.00258	0.00197	-0.00041	-0.00104	-0.00109	-0.00102	0.02512
(DLAR/DLPC)PC/P		-0.	-0.00100	-0.00352	-0.00335	-0.00320	-0.00061	-0.00101	-0.00239	-0.00251	-0.00237	-0.00211	0.01767
(DLCS/DLPC)PC/P		0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089	0.00089
(DLI/DHC)PC/P*		0.34617	0.35249	0.35042	0.32480	0.30433	0.29812	0.30520	0.33631	0.35673	0.36623	0.37404	0.37407
(DLT/DHC)PC/P*	0.63188	0.69410	0.72544	0.79342	0.79750	0.80130	0.73687	0.74862	0.80297	0.82289	0.83008	0.77767	0.36649
(DLAR/DHC)PC/P*		0.	0.01799	0.07353	0.10323	0.12750	0.08327	0.08562	0.09977	0.09685	0.09439	0.03416	-0.26417
(DLCS/DHC)PC/P*		0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947	0.36947
*(HC IN KCAL/G)													
(DLI/DLPCP)S		0.82848	0.50386	0.45325	0.42015	0.39370	0.36953	0.32873	0.17850	0.10158	0.06882	0.03547	0.02083
(DLT/DLPCP)S	-0.15730	-0.16781	-0.17332	-0.18581	-0.18678	-0.18768	-0.17586	-0.17801	-0.18842	-0.19247	-0.19411	-0.18185	-0.11130
(DLAR/DLPCP)S,		0.	0.32027	0.36093	0.39307	0.41862	0.45213	0.49118	0.63260	0.70592	0.73707	0.78267	0.84761

MOLE FRACTIONS

AL1CL1(G)	0.00018	0.00004	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	0.	0.	0.	0.	0.
AL1CL3(G)	0.00007	0.00004	0.00002	0.00002	0.00002	0.00002	0.00002	0.00001	0.	0.	0.	0.	0.
AL1O1CL1(G)	0.00064	0.00021	0.00009	0.00008	0.00008	0.00008	0.00008	0.00005	0.	0.	0.	0.	0.
C2H4(G)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.00192
C1O1(G)	0.26432	0.26358	0.26278	0.26253	0.26252	0.26250	0.26239	0.26196	0.25770	0.24751	0.23231	0.17527	0.11892
C1O2(G)	0.01780	0.01926	0.02034	0.02063	0.02063	0.02063	0.02076	0.02127	0.02581	0.03596	0.05100	0.10802	0.16249
C1O1S1(G)	0.00005	0.00005	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	0.00005	0.00004	0.00003	0.00002
CL1(G)	0.00176	0.00090	0.00056	0.00050	0.00052	0.00054	0.00052	0.00042	0.00007	0.	0.	0.	0.
H1(G)	0.00619	0.00309	0.00190	0.00168	0.00175	0.00182	0.00175	0.00141	0.00024	0.00001	0.	0.	0.
H2(G)	0.32142	0.32439	0.32599	0.32638	0.32636	0.32633	0.32651	0.32715	0.33209	0.34217	0.35702	0.41399	0.46288
H1CL1(G)	0.13179	0.13354	0.13415	0.13427	0.13424	0.13421	0.13425	0.13442	0.13497	0.13581	0.13695	0.13715	0.13586
H1C1O1(G)	0.00007	0.00003	0.00002	0.00002	0.00002	0.00002	0.00002	0.00001	0.	0.	0.	0.	0.
H2O1(G)	0.14646	0.14555	0.14472	0.14447	0.14445	0.14443	0.14430	0.14387	0.13964	0.12910	0.11335	0.05620	0.00782
H1S1(G)	0.00045	0.00033	0.00025	0.00023	0.00024	0.00025	0.00025	0.00022	0.00007	0.00001	0.	0.	0.
H2S1(G)	0.00153	0.00179	0.00193	0.00196	0.00194	0.00193	0.00193	0.00199	0.00224	0.00233	0.00234	0.00236	0.00238
MG1(G)	0.00007	0.00003	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.	0.	0.	0.	0.
MG1CL1(G)	0.00001	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
MG1CL2(G)	0.00101	0.00108	0.00109	0.00110	0.00109	0.00109	0.00109	0.00110	0.00111	0.00072	0.00011	0.	0.
MG1H1(G)	0.00001	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
N2(G)	0.06830	0.06847	0.06854	0.06855	0.06855	0.06855	0.06855	0.06857	0.06864	0.06862	0.06858	0.06857	0.06905
N1O1(G)	0.00003	0.00001	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
O1(G)	0.00001	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
O1H1(G)	0.00076	0.00029	0.00015	0.00013	0.00013	0.00014	0.00013	0.00009	0.00001	0.	0.	0.	0.
S1(G)	0.00010	0.00005	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.	0.	0.	0.	0.
S1O1(G)	0.00017	0.00011	0.00007	0.00006	0.00007	0.00007	0.00007	0.00006	0.00001	0.	0.	0.	0.
S1O2(G)	0.00007	0.00005	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00001	0.	0.	0.	0.
MG1O1(S)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.00039	0.00100	0.00111	0.
MG1CL2(S)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.00112
AL2O3(S)	0.	0.	0.	0.00191	0.01702	0.03093	0.03723	0.03726	0.03733	0.03733	0.03730	0.03730	0.03756
AL2O3(L)	0.03671	0.03710	0.03722	0.03532	0.02021	0.00630	0.	0.	0.	0.	0.	0.	0.

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDITIONS

AL1(G)	AL1O1(G)	C1H3(G)	C2H2(G)	C2N2(G)	CL2(G)	CL1O1(G)	MG1O1(G)	MG1O1H1(G)	N1H1(G)
N1O2(G)	O2(G)	S1O3(G)	S1(S)	MG1CL2(L)	MG1(S)	MG1(L)	C1(S)	AL1(S)	AL1(L)

PRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM CALCULATIONS

AL2(G)	AL1H1(G)	AL2O1(G)	AL2O2(G)	C1(G)	C2(G)	C3(G)	C1CL1(G)	C1CL4(G)	C1H1(G)
C1H2(G)	C1H4(G)	C1N1(G)	C1O1CL2(G)	C1S1(G)	C1S2(G)	CL1C1N1(G)	CL1O2(G)	CL2O1(G)	H1C1N1(G)
MG1S1(G)	N1(G)	N1H3(G)	N2O1(G)	N1S1(G)	S2(G)	S1CL1(G)	S1CL2(G)	S2CL2(G)	S1O1CL1(G)
S1O1CL2(G)									

INPUT, G-ATOMS/G

	N	H	CL	O	C	S	AL	MG
FUEL	0.6132922E-02	0.4839509E-01	0.6132922E-02	0.2506609E-01	0.1266924E-01	0.1066117E-03	0.3335804E-02	0.4960317E-04
OXIDANT	0.	0.	0.	0.	0.	0.	0.	0.
PROPELLANT	0.6132922E-02	0.4839509E-01	0.6132922E-02	0.2506609E-01	0.1266924E-01	0.1066117E-03	0.3335804E-02	0.4960317E-04

CASE NO. 51 500.0 0.

TABLE XI. - THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

CASE NO. 51 500.0 0.

	CHEMICAL FORMULA				WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 1.00000	H 4.00000	CL 1.00000	O 4.00000	0.72060	-70730.000	S	298.15	-0.
FUEL	H 1.86955	O 0.03126	C 1.00000	S 0.00841	0.18580	-2999.082	L	298.15	-0.
FUEL	AL 1.00000				0.09000	0.	S	298.15	-0.
FUEL	O 1.00000	MG 1.00000			0.00200	-143700.000	S	298.15	-0.
FUEL	H 2.00000	O 1.00000			0.00160	-68317.399	L	298.15	-0.

O/F= 0. , PERCENT FUEL=100.0000, EQUIVALENCE RATIO= 1.9480, DENSITY= 0.

PARAMETERS

	CHAMBER	THROAT	EXIT	EXIT
PC/P	1.000	1.788	2.500	2.750
P, ATM	34.02	19.02	13.61	12.37
T, DEG K	2737	2459	2311	2270
H, CAL/G	-485.0	-614.6	-683.3	-702.0
S, CAL/(G)(K)	2.5264	2.5264	2.5264	2.5264
M, MOL WT	23.126	23.126	23.126	23.126
CP, CAL/(G)(K)	0.4699	0.4641	0.4605	0.4594
GAMMA	1.2238	1.2272	1.2294	1.2301
MACH NUMBER	0.	1.000	1.275	1.345
CSTAR, FT/SEC		4980	4980	4980
CF		0.686	0.849	0.888
AE/AT		1.000	1.062	1.097
IVAC,LB-SEC/LB		192.8	197.1	199.2
I, LB-SEC/LB ,		106.2	131.4	137.4

MOLE FRACTIONS

AL1CL1(G)	0.00018	AL1CL3(G)	0.00007	AL1O1CL1(G)	0.00064	C1O1(G)	0.26432
C1O2(G)	0.01780	C1O1S1(G)	0.00005	CL1(G)	0.00176	H1(G)	0.00619
H2(G)	0.32142	H1CL1(G)	0.13179	H1C1O1(G)	0.00007	H2O1(G)	0.14646
H1S1(G)	0.00045	H2S1(G)	0.00153	MG1(G)	0.00007	MG1CL1(G)	0.00001
MG1CL2(G)	0.00101	MG1H1(G)	0.00001	N2(G)	0.06830	N1O1(G)	0.00003
O1(G)	0.00001	O1H1(G)	0.00076	S1(G)	0.00010	S1O1(G)	0.00017
S1O2(G)	0.00007	AL2O3(L)	0.03671				

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDITIONS

AL1(G)	AL1O1(G)	C1H3(G)	C2H2(G)	C2H4(G)	C2N2(G)	CL2(G)	CL1O1(G)	MG1O1(G)	MG1O1H1(G)
N1H1(G)	N1O2(G)	O2(G)	S1O3(G)	S1(S)	MG1O1(S)	MG1CL2(S)	MG1CL2(L)	MG1(S)	MG1(L)
C1(S)	AL2O3(S)	AL1(S)	AL1(L)						

PRODUCTS WHICH WERE INTENTIONALLY OMITTED FROM CALCULATIONS

AL2(G)	AL1H1(G)	AL2O1(G)	AL2O2(G)	C1(G)	C2(G)	C3(G)	C1CL1(G)	C1CL4(G)	C1H1(G)
C1H2(G)	C1H4(G)	C1N1(G)	C1O1CL2(G)	C1S1(G)	C1S2(G)	CL1C1N1(G)	CL1O2(G)	CL2O1(G)	H1C1N1(G)
MG1S1(G)	N1(G)	N1H3(G)	N2O1(G)	N1S1(G)	S2(G)	S1CL1(G)	S1CL2(G)	S2CL2(G)	S1O1CL1(G)
S1O1CL2(G)									

INPUT, G-ATOMS/G

	N	H	CL	O	C	S	AL	MG
FUEL	0.6132922E-02	0.4839509E-01	0.6132922E-02	0.2506609E-01	0.1266924E-01	0.1066117E-03	0.3335804E-02	0.4960317E-04
OXIDANT	0.	0.	0.	0.	0.	0.	0.	0.
PROPELLANT	0.6132922E-02	0.4839509E-01	0.6132922E-02	0.2506609E-01	0.1266924E-01	0.1066117E-03	0.3335804E-02	0.4960317E-04

CASE NO. 51 500.0 0.

TABLE XII. - THEORETICAL THERMODYNAMIC PROPERTIES AT ASSIGNED PRESSURE AND TEMPERATURES

CASE NO. 50 0.1 34.293

	CHEMICAL FORMULA				WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H 2.00000				1.00000	0.	G	298.15	-0.
OXIDANT	N 0.78088	O 0.20979	AR 0.00466	C 0.00015	1.00000	-7.202	G	298.15	-0.

O/F=34.292881, PERCENT FUEL= 2.8334, EQUIVALENCE RATIO= 1.0000, DENSITY= 0.

EQUILIBRIUM THERMODYNAMIC PROPERTIES

P, ATM	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100	0.0100
T, DEG K	6000	5500	5000	4500	4000	3500	3000	2500	2000	1500	1000	500	300
H, CAL/G	10068.8	8048.6	5825.5	4546.9	3967.9	3595.5	2656.3	570.8	-165.4	-407.4	-590.0	-752.2	-812.3
S, CAL/(G)(K)	5.5853	5.2324	4.8097	4.5420	4.4066	4.3071	4.0119	3.2550	2.9351	2.7976	2.6502	2.4269	2.2737
M, MOL WT	10.995	11.982	13.337	14.192	14.519	14.735	16.261	22.053	24.416	24.641	24.648	24.648	24.648
(DLM/DLP)T	0.03312	0.05700	0.03807	0.01340	0.00470	0.01138	0.07459	0.04710	0.00354	0.00009	0.	0.	0.
(DLM/DLT)P	-0.6567	-1.2242	-0.8918	-0.3391	-0.1041	-0.1834	-1.4100	-1.1183	-0.1098	-0.0036	-0.	-0.	-0.
CP, CAL/(G)(K)	2.8811	4.8553	3.5858	1.6743	0.8065	0.8612	3.7142	2.8329	0.6812	0.3899	0.3449	0.3052	0.2968
GAMMA	1.1615	1.1261	1.1244	1.1582	1.2535	1.2625	1.1319	1.1057	1.1677	1.2630	1.3050	1.3591	1.3730

MOLE FRACTIONS

AR1(G)	0.00344	0.00375	0.00417	0.00444	0.00454	0.00461	0.00509	0.00690	0.00764	0.00771	0.00771	0.00771	0.00771
C1(G)	0.00009	0.00005	0.00001	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.
C1O1(G)	0.00002	0.00007	0.00013	0.00014	0.00015	0.00015	0.00016	0.00015	0.00004	0.	0.	0.	0.
C1O2(G)	0.	0.	0.	0.	0.	0.	0.00001	0.00007	0.00021	0.00025	0.00025	0.00025	0.00025
H1(G)	0.30905	0.33678	0.37477	0.39852	0.40622	0.40080	0.32001	0.06585	0.00186	0.	0.	0.	0.
H2(G)	0.	0.00001	0.00003	0.00013	0.00065	0.00463	0.04138	0.06921	0.01318	0.00047	0.	0.	0.
H2O1(G)	0.	0.	0.	0.	0.	0.00010	0.01174	0.18877	0.32669	0.34582	0.34642	0.34642	0.34642
N1(G)	0.48942	0.35411	0.16863	0.05223	0.01071	0.00135	0.00009	0.	0.	0.	0.	0.	0.
N2(G)	0.04323	0.13665	0.26467	0.34495	0.37371	0.38279	0.42085	0.57403	0.63898	0.64544	0.64563	0.64562	0.64562
N1H1(G)	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.	0.	0.	0.	0.	0.	0.
N1O1(G)	0.00012	0.00031	0.00070	0.00134	0.00248	0.00502	0.01008	0.00726	0.00113	0.00004	0.	0.	0.
O1(G)	0.15462	0.16825	0.18684	0.19808	0.20077	0.19503	0.14349	0.02335	0.00047	0.	0.	0.	0.
O2(G)	0.	0.	0.00001	0.00003	0.00018	0.00159	0.01627	0.02631	0.00509	0.00020	0.	0.	0.
O1H1(G)	0.	0.00001	0.00003	0.00012	0.00058	0.00393	0.03084	0.03810	0.00472	0.00008	0.	0.	0.

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.000005 FOR ALL ASSIGNED CONDITIONS

C2(G)	C3(G)	C1H1(G)	C1H2(G)	C1H3(G)	C1H4(G)	C2H2(G)	C2H4(G)	C1N1(G)	C2N2(G)
H1C1N1(G)	H1C1O1(G)	N1H3(G)	N1O2(G)	N2O1(G)	C1(S)				

INPUT, G-ATOMS/G

	H	N	O	AR	C
FUEL	0.9920635E 00	0.	0.	0.	0.
OXIDANT	0.	0.5391588E-01	0.1448528E-01	0.3218875E-03	0.1035674E-04
PROPELLANT	0.2810945E-01	0.5238821E-01	0.1407485E-01	0.3127670E-03	0.1006329E-04

CASE NO. 50 0.1 34.293

TABLE XIII. - DETONATION PROPERTIES OF AN IDEAL REACTING GAS

CASE NO. 52 14.70 298.15

	CHEMICAL FORMULA	WT FRACTION	ENTHALPY CAL/MOL	STATE	TEMP DEG K	HEAT CAPACITY CAL/MOL-DEG K
FUEL	H 2	1.00000	0.	G	298.15	6.8922
OXIDANT	O 2	1.00000	0.	G	298.15	7.0215

O/F= 7.936508, PERCENT FUEL= 11.1901, EQUIVALENCE RATIO= 1.0000

THERMODYNAMIC PROPERITES

	UNBURNED GAS	BURNED GAS
P, ATM	1.00000	18.82775
T, DEG K	298.1	3682.1
H, CAL/G	0.	678.9
S, CAL/G-DEG K		4.1602
M, MOL. WT.	12.011	14.485
CP, CAL/G-DEG K	0.5774	3.9127
(DLNM/DLNP)T	0.	0.08280
(DLNM/DLNT)P	0.	-1.3715
GAMMA	1.4016	1.1292
US, M/SEC	537.9	1544.9

BURNED GAS COMPOSITION IN MOLE FRACTIONS

H1(G)	0.08124	H2(G)	0.16326	H2O1(G)	0.53167	O1(G)	0.03848
O2(G)	0.04849	O1H1(G)	0.13685				

DETONATION PARAMETERS (UD IN M/SEC, H1 IN KCAL/G)

P/P1 = 18.828	(DL(P/P1)/DLP1)T1,H1= 0.03783	(DL(P/P1)/DLT1)P1=-1.04086	(DL(P/P1)/DH1)P1,T1= 0.19925
T/T1 = 12.350	(DL(T/T1)/DLP1)T1,H1= 0.05178	(DL(T/T1)/DLT1)P1=-1.04234	(DL(T/T1)/DH1)P1,T1= 0.08883
UD = 2840.4	(D UD/DLP1)T1,H1 = 55.10	(D UD/DLT1)P1 = -95.85	(D UD/DH1)P1,T1 = 290.22
M/M1 = 1.2060			
RHO/RHO1= 1.8386			
MACH NO.= 5.2809			

INPUT, G-ATOMS/G

	H	O
FUEL	0.9920635E 00	0.
OXIDANT	0.	0.6250000E-01
PROPELLANT	0.1110124E-00	0.5550622E-01

CASE NO. 52 14.70 298.15

TABLE XIV. - PRELIMINARY OUTPUT

INPUT

N	1.0000	H	4.0000	CL	1.0000	O	4.0000	-0.	72.0600	-70730.00	S	298.150	F	0	0.	Read in from fuel and oxidant cards (see Table IX)
C	1.0000	H	1.8695	O	0.0313	S	0.0084	-0.	18.5800	-2999.08	L	298.150	F	1	0.	
AL	1.0000		-0.		-0.		-0.	-0.	9.0000	0.	S	298.150	F	0	0.	
MG	1.0000	O	1.0000		-0.		-0.	-0.	0.2000	143700.00	S	298.150	F	0	0.	
H	2.0000	O	1.0000		-0.		-0.	-0.	0.1600	-68317.40	L	298.150	F	0	0.	

OXIDANT	0.	0.		-0.	h_x, V_x^+, V_x^-
FUEL	-0.484973E 03	0.109605E-00		-0.562651E-01	h_f, V_f^+, V_f^-
N	0.		0.61329225E-02		$(b_x^o)_i$, $(b_f^o)_i$
H	0.		0.48395094E-01		
CL	0.		0.61329225E-02		
O	0.		0.25066092E-01		
C	0.		0.12669243E-01		
S	0.		0.10661168E-03		
AL	0.		0.33358043E-02		
MG	0.		0.49603175E-04		

51	H,S						Case number, problem type
0.	0.09999999E 03	0.19480125E 01	0.50000000E 03				O/F, %F, ℛ, P_c
-0.48497294E 03	0.61329225E-02	0.48395094E-01	0.61329225E-02	0.25066092E-01	0.12669243E-01	0.10661168E-03	h_0, b_i^o (i = 1, 2, . . ., 6)
0.33358043E-02	0.49603175E-04						b_i^o (i = 7, 8)

THE SPECIES AL2O3(L) HAS NO DATA AT T= 2269.8

Printed during frozen expansion calculation

TABLE XV. - INTERMEDIATE OUTPUT

(a) Example of first iteration for combustion conditions for problem in Table X.

```
 51    H,S                                                                                                               Case number, problem type
 0.                 0.99999999E 03   0.19480125E 01   0.50000000E 03                                                      O/F, %F, r, Pc
-0.48497294E 03    0.61329225E-02   0.48395094E-01   0.61329225E-02   0.25066092E-01   0.12669243E-01   0.10661168E-03  h0, b°i (i = 1, 2, . . ., 6)
 0.33358043E-02    0.49603175E-04                                                                                     b°i (i = 7, 8)
0.110000E 02  0.100000E 01  0.            0.300000E 01  0.400000E 01  0.            0.            0.
0.            0.700000E 01  0.733718E 02 -0.215544E 03  0.
0.100000E 01  0.490000E 02  0.100000E 01  0.500000E 01  0.160000E 02  0.300000E 01  0.            0.200000E 01
0.            0.230000E 02  0.194079E 03 -0.729533E 03  0.
0.            0.100000E 01  0.230000E 02  0.200000E 01  0.            0.            0.500000E 01  0.300000E 01
0.            0.130000E 02 -0.157641E 02 -0.615408E 03  0.
0.300000E 01  0.500000E 01  0.200000E 01  0.380000E 02  0.500000E 01  0.700000E 01  0.200000E 01  0.200000E 01
0.300000E 01  0.240000E 02  0.481188E 02 -0.969240E 03  0.
0.400000E 01  0.160000E 02  0.            0.500000E 01  0.170000E 02  0.100000E 01  0.            0.
0.            0.110000E 02  0.110858E 03 -0.437513E 03  0.                                                            Iteration equations
0.            0.300000E 01  0.            0.700000E 01  0.100000E 01  0.700000E 01  0.            0.                   corresponding to Table I
0.            0.700000E 01  0.264634E 02 -0.265161E 03  0.
0.            0.            0.500000E 01  0.200000E 01  0.            0.            0.500000E 01  0.
0.200000E 01  0.500000E 01  0.684315E 01 -0.210814E 03 -0.904752E-08
0.            0.200000E 01  0.300000E 01  0.200000E 01  0.            0.            0.            0.600000E 01
0.            0.600000E 01  0.240722E 02 -0.210885E 03  0.
0.            0.            0.            0.300000E 01  0.            0.            0.200000E 01  0.
0.            0.           -0.344450E 02 -0.836849E 02  0.
0.700000E 01  0.230000E 02  0.130000E 02  0.240000E 02  0.110000E 02  0.700000E 01  0.500000E 01  0.600000E 01
0.            0.            0.198549E 03 -0.130039E 04 -0.117286E-07
0.733718E 02  0.194079E 03 -0.157641E 02  0.481188E 02  0.110858E 03  0.264634E 02  0.684315E 01  0.240722E 02
-0.344450E 02  0.198549E 03  0.274225E 04 -0.457419E 04 -0.133434E-07
-0.121137E 02 -0.866015E 01 -0.192444E 02 -0.164985E 02 -0.772146E 01 -0.169725E 02 -0.156589E 02 -0.175637E 02   Solutions to equa-
-0.216086E 01  0.901087E-01  0.833695E-01                                                                            tions of Table I
        0.38276260E 04            0.38999999E 02            0.14841316E 03            0.21348344E-00                 Current T, P, A, λ
       AL1(G)          0.100000E 01   0.            -0.911896E 00   0.124892E 02   0.261951E 02
OMIT   AL2(G)          0.             0.             0.             0.             0.
       AL1CL1(G)       0.100000E 01   0.             0.149154E 01   0.275359E 01   0.389189E 02
       AL1CL3(G)       0.100000E 01   0.            -0.239042E 01  -0.915783E 01   0.626075E 02
OMIT   AL1H1(G)        0.             0.             0.             0.             0.
       AL1O1(G)        0.100000E 01   0.            -0.681145E 00   0.634502E 01   0.372923E 02
OMIT   AL2O1(G)        0.             0.             0.             0.             0.
OMIT   AL2O2(G)        0.             0.             0.             0.             0.
       AL1O1CL1(G)     0.100000E 01   0.             0.185817E 01  -0.558687E 01   0.481389E 02
OMIT   C1(G)           0.             0.             0.             0.             0.
OMIT   C2(G)           0.             0.             0.             0.             0.
OMIT   C3(G)           0.             0.             0.             0.             0.
OMIT   C1CL1(G)        0.             0.             0.             0.             0.
OMIT   C1CL4(G)        0.             0.             0.             0.             0.
OMIT   C1H1(G)         0.             0.             0.             0.             0.
OMIT   C1H2(G)         0.             0.             0.             0.             0.
       C1H3(G)         0.100000E 01   0.            -0.288955E 01   0.120906E 02   0.418950E 02
OMIT   C1H4(G)         0.             0.             0.             0.             0.
       C2H2(G)         0.100000E 01   0.            -0.185501E 01   0.157945E 02   0.453860E 02
       C2H4(G)         0.100000E 01   0.            -0.783302E 01   0.138526E 02   0.549482E 02
OMIT   C1N1(G)         0.             0.             0.             0.             0.
       C2N2(G)         0.100000E 01   0.            -0.462276E 01   0.186688E 02   0.521600E 02
       C1O1(G)         0.100000E 01   0.             0.936841E 01   0.437705E-00   0.339895E 02
       C1O2(G)         0.100000E 01   0.             0.672690E 01  -0.593632E 01   0.420039E 02
OMIT   C1O1CL2(G)      0.             0.             0.             0.             0.
       C1O1S1(G)       0.100000E 01   0.             0.164919E 01   0.233114E 01   0.449784E 02
OMIT   C1S1(G)         0.             0.             0.             0.             0.
OMIT   C1S2(G)         0.             0.             0.             0.             0.
       CL1(G)          0.100000E 01   0.             0.166865E 01   0.619662E 01   0.265931E 02
       CL2(G)          0.100000E 01   0.            -0.410049E 01   0.422851E 01   0.382644E 02
OMIT   CL1C1N1(G)      0.             0.             0.             0.             0.
       CL1O1(G)        0.100000E 01   0.            -0.408197E 01   0.733451E 01   0.383840E 02
OMIT   CL1O2(G)        0.             0.             0.             0.             0.
OMIT   CL2O1(G)        0.             0.             0.             0.             0.
       H1(G)           0.100000E 01   0.             0.311313E 01   0.915493E 01   0.201650E 02
       H2(G)           0.100000E 01   0.             0.471037E 01   0.375050E 01   0.254685E 02
       H1CL1(G)        0.100000E 01   0.             0.370726E 01   0.954479E 00   0.324868E 02
OMIT   H1C1N1(G)       0.             0.             0.             0.             0.
       H1C1O1(G)       0.100000E 01   0.             0.365572E 01   0.530283E 01   0.413965E 02
       H2O1(G)         0.100000E 01   0.             0.426280E 01  -0.211712E 01   0.361409E 02
       H1S1(G)         0.100000E 01   0.             0.329342E-00   0.872168E 01   0.339565E 02
       H2S1(G)         0.100000E 01   0.             0.764277E-01   0.520129E 01   0.391369E 02
       MG1(G)          0.100000E 01   0.             0.284469E-00   0.700552E 01   0.242697E 02
       MG1CL1(G)       0.100000E 01   0.            -0.130882E 01   0.442983E 01   0.395599E 02
       MG1CL2(G)       0.100000E 01   0.            -0.611901E 00  -0.641490E 01   0.495606E 02
       MG1H1(G)        0.100000E 01   0.            -0.842651E 00   0.953103E 01   0.341177E 02
       MG1O1(G)        0.100000E 01   0.            -0.163339E 01   0.529269E 01   0.372802E 02
       MG1O1H1(G)      0.100000E 01   0.            -0.242100E 01   0.422804E 01   0.441769E 02
OMIT   MG1S1(G)        0.             0.             0.             0.             0.
OMIT   N1(G)           0.             0.             0.             0.             0.
       N2(G)           0.100000E 01   0.             0.539068E 01   0.388045E 01   0.331750E 02
       N1H1(G)         0.100000E 01   0.            -0.203844E 01   0.142380E 02   0.317864E 02
OMIT   N1H3(G)         0.             0.             0.             0.             0.
       N1O1(G)         0.100000E 01   0.             0.901690E 00   0.680628E 01   0.357527E 02
       N1O2(G)         0.100000E 01   0.            -0.711965E 01   0.722893E 01   0.446172E 02
OMIT   N2O1(G)         0.             0.             0.             0.             0.
OMIT   N1S1(G)         0.             0.             0.             0.             0.
       O1(G)           0.100000E 01   0.             0.186372E-01   0.101553E 02   0.258257E 02
       O2(G)           0.100000E 01   0.            -0.139659E 01   0.414033E 01   0.353955E 02
       O1H1(G)         0.100000E 01   0.             0.221818E 01   0.500759E 01   0.319669E 02
       S1(G)           0.100000E 01   0.            -0.261229E-00   0.111543E 02   0.269356E 02
OMIT   S2(G)           0.             0.             0.             0.             0.
OMIT   S1CL1(G)        0.             0.             0.             0.             0.
OMIT   S1CL2(G)        0.             0.             0.             0.             0.
OMIT   S2CL2(G)        0.             0.             0.             0.             0.
       S1O1(G)         0.100000E 01   0.             0.172176E-00   0.425293E 01   0.375415E 02
       S1O2(G)         0.100000E 01   0.            -0.107387E 01  -0.305684E 01   0.460935E 02
       S1O3(G)         0.100000E 01   0.            -0.850698E 01  -0.214113E 01   0.559982E 02
OMIT   S1O1CL1(G)      0.             0.             0.             0.             0.
OMIT   S1O1CL2(G)      0.             0.             0.             0.             0.
       S1(S)           0.             0.             0.             0.             0.
       MG1O1(S)        0.             0.             0.             0.             0.
       MG1CL2(S)       0.             0.             0.             0.             0.
       MG1CL2(L)       0.             0.             0.             0.             0.
       MG1(S)          0.             0.             0.             0.             0.
       MG1(L)          0.             0.             0.             0.             0.
       C1(S)           0.             0.             0.             0.             0.
       AL2O3(S)        0.             0.             0.             0.             0.
       AL2O3(L)        0.             0.            -0.216086E 01  -0.344450E 02   0.492399E 02
       AL1(S)          0.             0.             0.             0.             0.
       AL1(L)          0.             0.             0.             0.             0.
```

TABLE XV. - Concluded. INTERMEDIATE OUTPUT

(b) Example of converged data at throat for problem in Table X.

PC/P	P, ATM	T, DEG K	H, CAL/G	S, CAL/(G)(K)
M, MOL WT	CP, CAL/(G)(K)	(DLM/DLP)T	(DLM/DLT)P	GAMMA
AE/AT	MACH NUMBER	I, LB-SEC/LB	IVAC, LB-SEC/LB	CSTAR, FT/SEC
(DLT/DLPC)PC/P	(DLI/DLPC)PC/P	(DLAR/DLPC)PC/P	(DL(A/W)/DLPC)PC/P	(DLCS/DLPC)PC/P
(DLT/DHC)PC/P	(DLI/DHC)PC/P	(DLAR/DHC)PC/P	(DL(A/W)/DHC)PC/P	(DLCS/DHC)PC/P
(DLT/DLPCP)S	(DLI/DLPCP)S	(DLAR/DLPCP)S	(DL(A/W)/DLPCP)S	(DLCS/DLPCP)S

0.17766215E 01	0.19150352E 02	0.24923622E 04	-0.61386123E 03	0.25264481E 01
0.23192056E 02	0.52646955E 00	0.14729141E-02	-0.31039675E-01	0.12070672E 01
0.09999999E 01	0.99998981E 00	0.10590088E 03	0.19363671E 03	0.50150601E 04
0.67940462E 00	0.	0.	0.	
0.45872999E-02	0.23652089E-02	-0.	-0.99910843E 00	0.89157373E-03
0.69409923E 00	0.34617421E-00	0.	0.36946963E-00	0.36946963E-00
-0.16780989E-00	0.82848097E 00	0.	0.	0.

	AL1(G)	0.	OMIT	AL2(G)	0.		AL1CL1(G)	0.00004
	AL1CL3(G)	0.00004	OMIT	AL1H1(G)	0.		AL1O1(G)	0.
OMIT	AL2O1(G)	0.	OMIT	AL2O2(G)	0.		AL1O1CL1(G)	0.00021
OMIT	C1(G)	0.	OMIT	C2(G)	0.	OMIT	C3(G)	0.
OMIT	C1CL1(G)	0.	OMIT	C1CL4(G)	0.	OMIT	C1H1(G)	0.
OMIT	C1H2(G)	0.		C1H3(G)	0.	OMIT	C1H4(G)	0.
	C2H2(G)	0.		C2H4(G)	0.	OMIT	C1N1(G)	0.
	C2N2(G)	0.		C1O1(G)	0.26358		C1O2(G)	0.01926
OMIT	C1O1CL2(G)	0.		C1O1S1(G)	0.00005	OMIT	C1S1(G)	0.
OMIT	C1S2(G)	0.		CL1(G)	0.00090		CL2(G)	0.
OMIT	CL1C1N1(G)	0.		CL1O1(G)	0.	OMIT	CL1O2(G)	0.
OMIT	CL2O1(G)	0.		H1(G)	0.00309		H2(G)	0.32439
	H1CL1(G)	0.13354	OMIT	H1C1N1(G)	0.		H1C1O1(G)	0.00003
	H2O1(G)	0.14555		H1S1(G)	0.00033		H2S1(G)	0.00179
	MG1(G)	0.00003		MG1CL1(G)	0.		MG1CL2(G)	0.00108
	MG1H1(G)	0.		MG1O1(G)	0.		MG1O1H1(G)	0.
OMIT	MG1S1(G)	0.	OMIT	N1(G)	0.		N2(G)	0.06847
	N1H1(G)	0.	OMIT	N1H3(G)	0.		N1O1(G)	0.00001
	N1O2(G)	0.	OMIT	N2O1(G)	0.	OMIT	N1S1(G)	0.
	O1(G)	0.		O2(G)	0.		O1H1(G)	0.00029
	S1(G)	0.00005	OMIT	S2(G)	0.	OMIT	S1CL1(G)	0.
OMIT	S1CL2(G)	0.	OMIT	S2CL2(G)	0.		S1O1(G)	0.00011
	S1O2(G)	0.00005		S1O3(G)	0.	OMIT	S1O1CL1(G)	0.
OMIT	S1O1CL2(G)	0.		S1(S)	0.		MG1O1(S)	0.
	MG1CL2(S)	0.		MG1CL2(L)	0.		MG1(S)	0.
	MG1(L)	0.		C1(S)	0.		AL2O3(S)	0.
	AL2O3(L)	0.03710		AL1(S)	0.		AL1(L)	0.

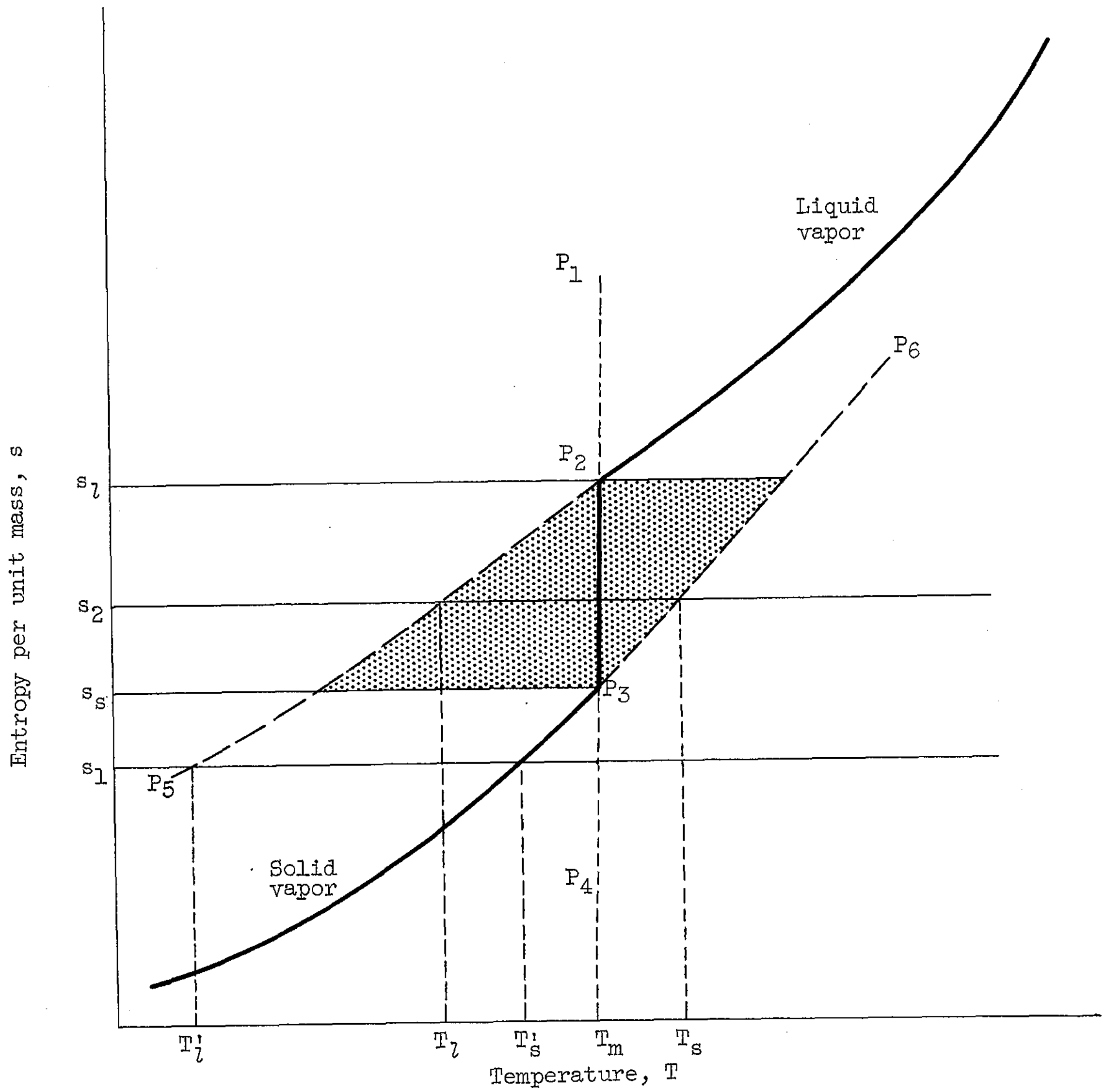


Figure 1. - System entropy as function of temperature and constant system pressure in vicinity of melting point.

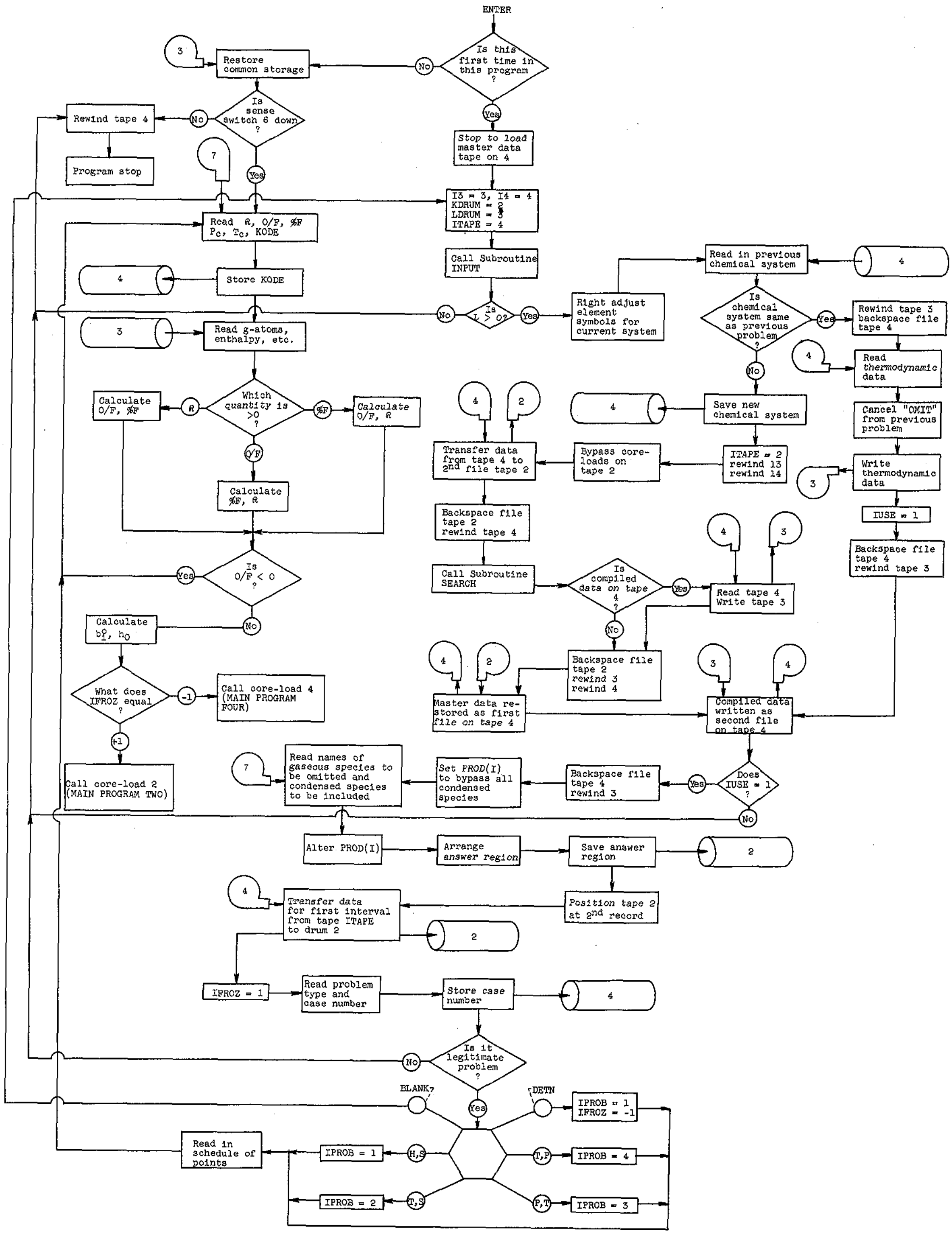


Figure 2. - MAIN PROGRAM ONE (input program).

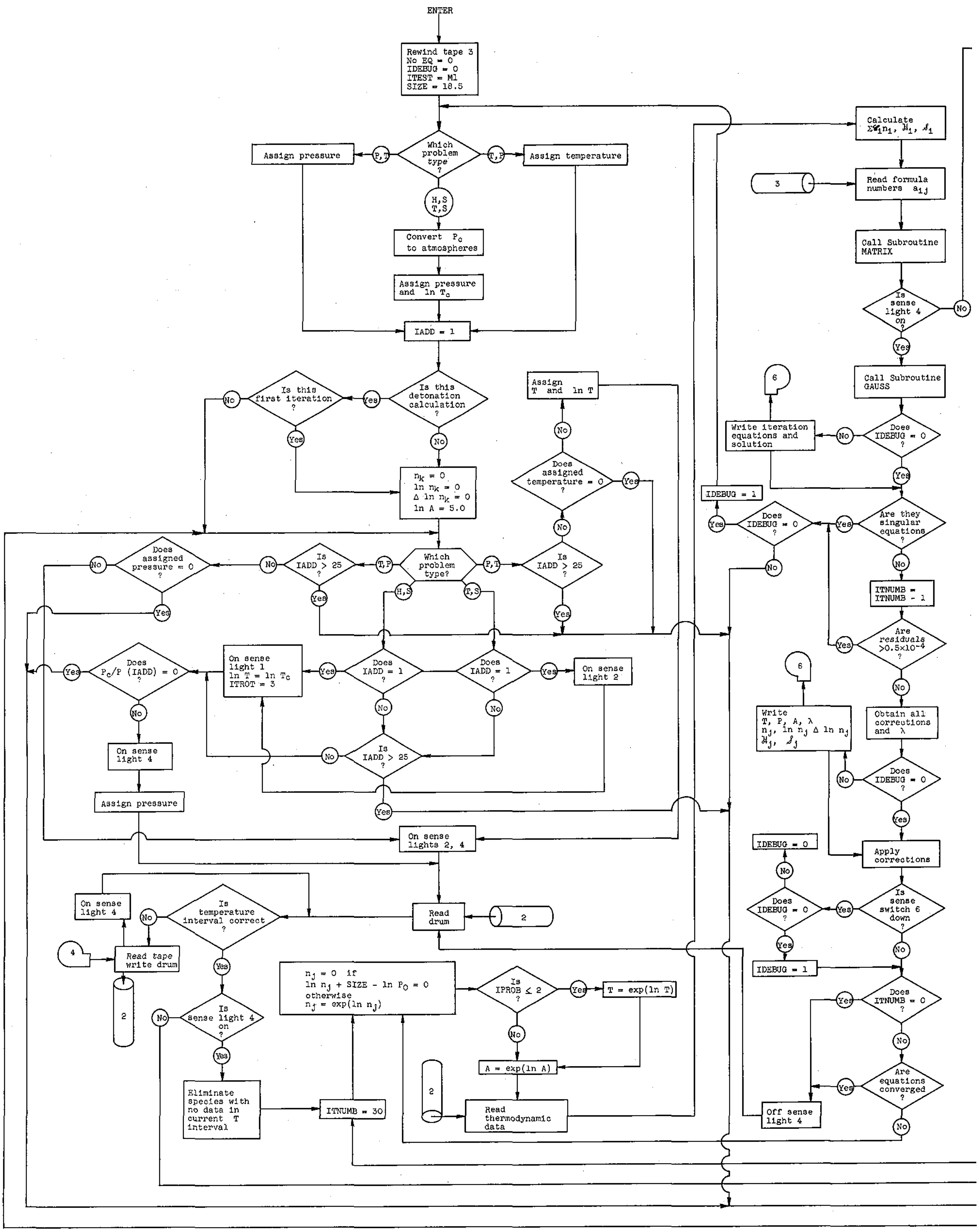
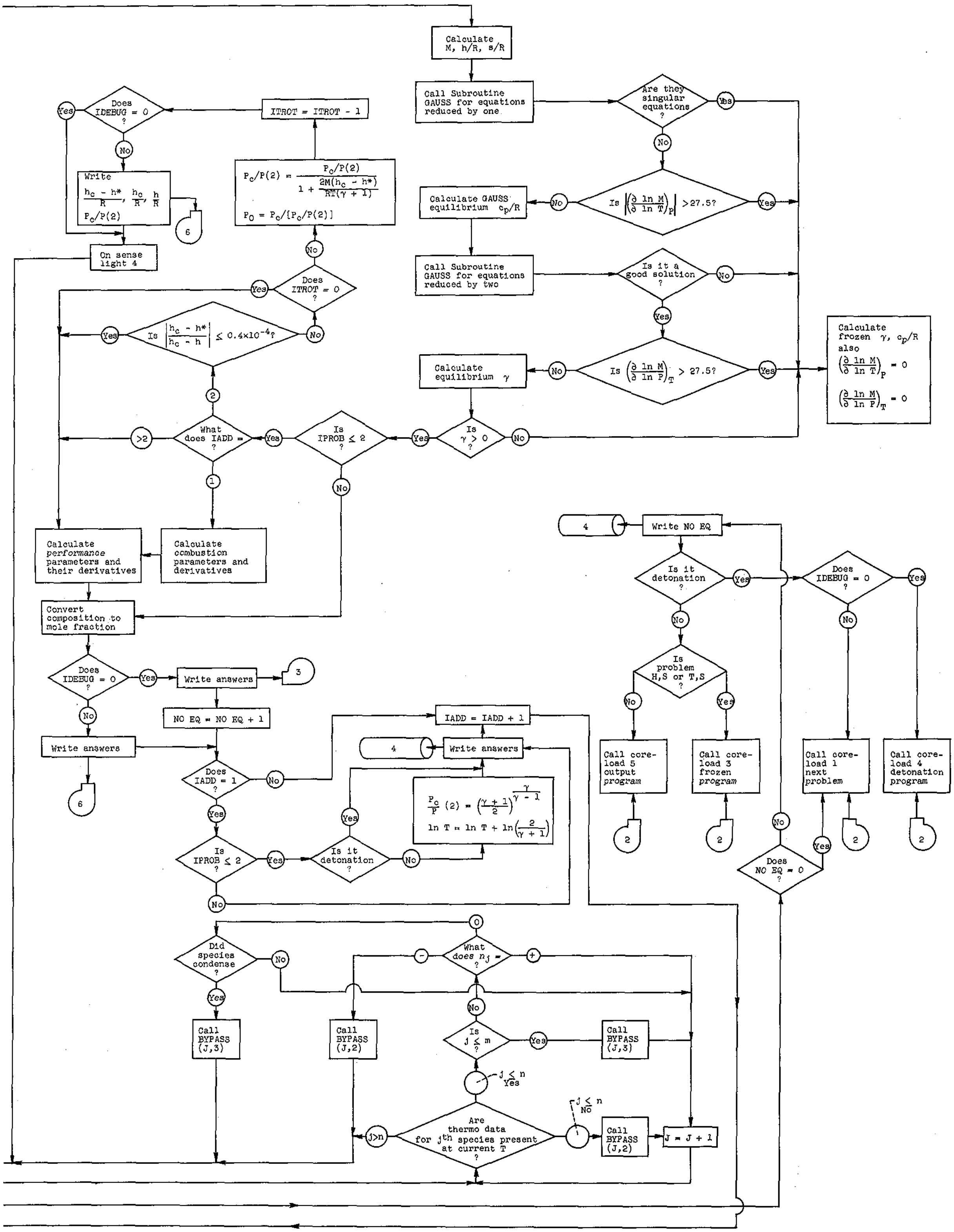


Figure 3. - MAIN PROGRAM TWO (chemical



equilibrium computations).

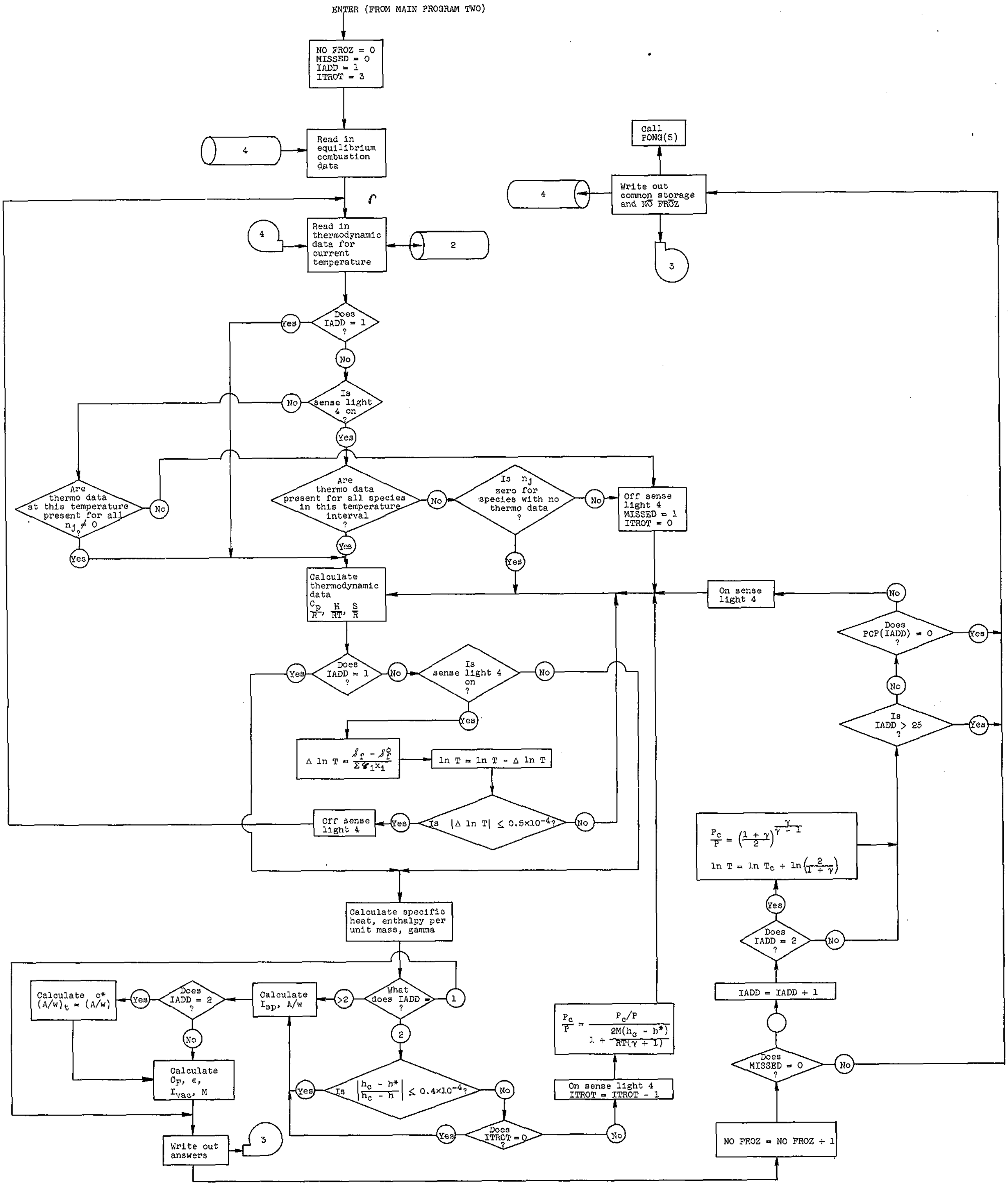


Figure 4. - MAIN PROGRAM THREE (frozen composition expansion).

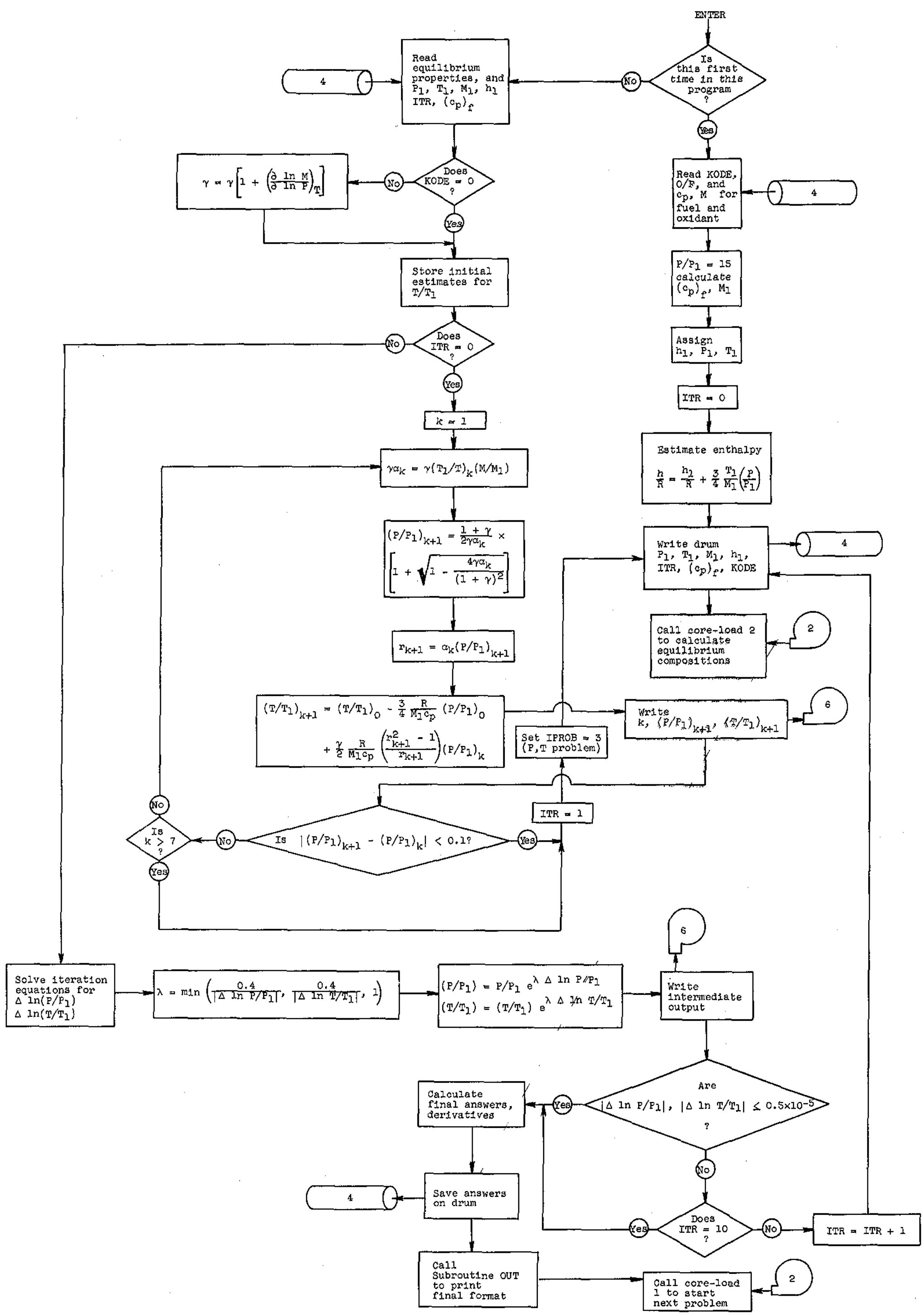
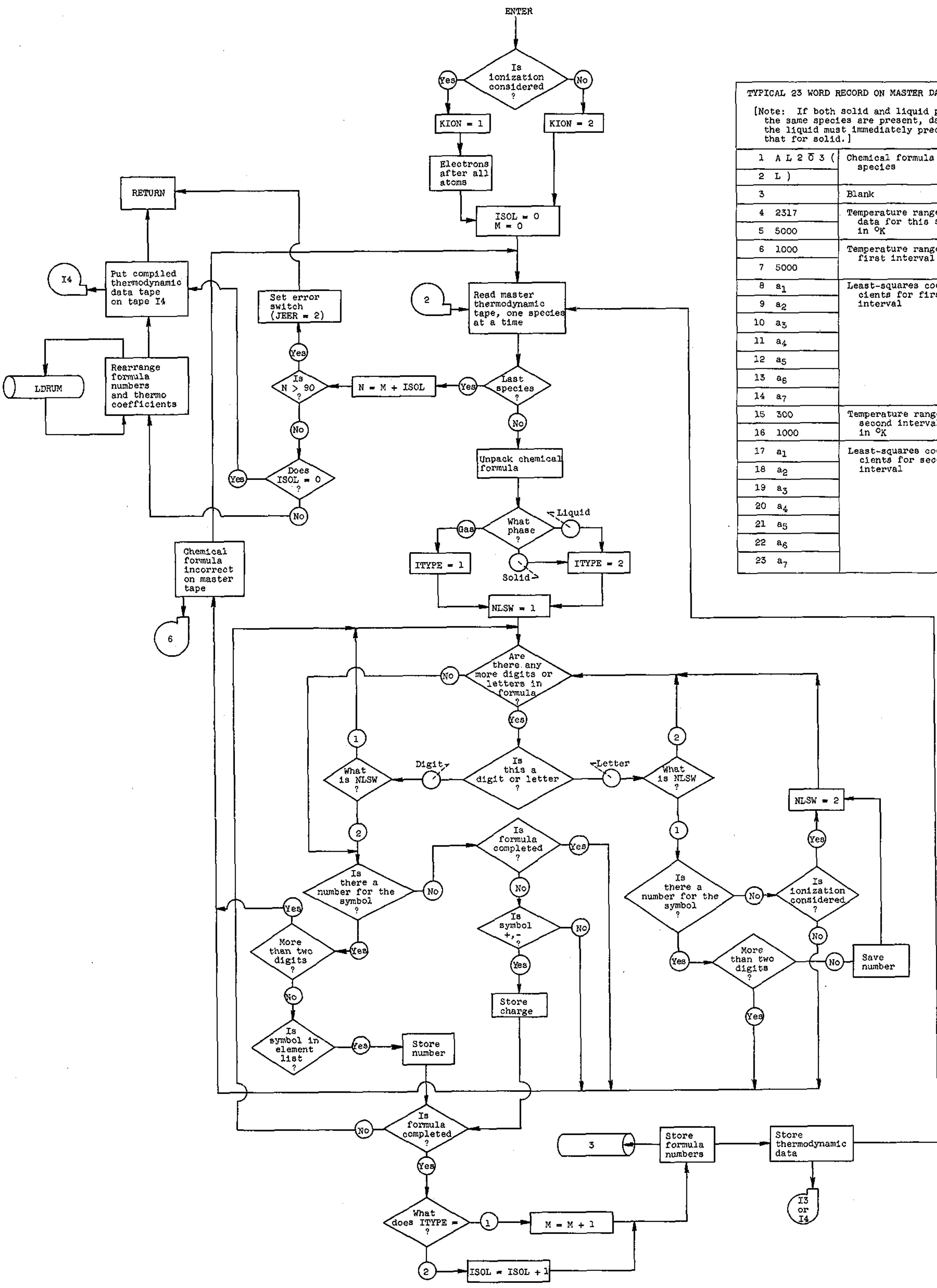


Figure 5. - MAIN PROGRAM FOUR (Chapman-Jouguet detonations).



TYPICAL 23 WORD RECORD ON MASTER DATA TAPE

[Note: If both solid and liquid phase of the same species are present, data for the liquid must immediately precede that for solid.]

1	A L 2 Ō 3 (	Chemical formula for species
2	L)	
3		Blank
4	2317	Temperature range of data for this species in °K
5	5000	
6	1000	Temperature range for first interval in °K
7	5000	
8	a_1	Least-squares coefficients for first interval
9	a_2	
10	a_3	
11	a_4	
12	a_5	
13	a_6	
14	a_7	
15	300	Temperature range for second interval in °K
16	1000	
17	a_1	Least-squares coefficients for second interval
18	a_2	
19	a_3	
20	a_4	
21	a_5	
22	a_6	
23	a_7	

Figure 6. - Subroutine SEARCH.

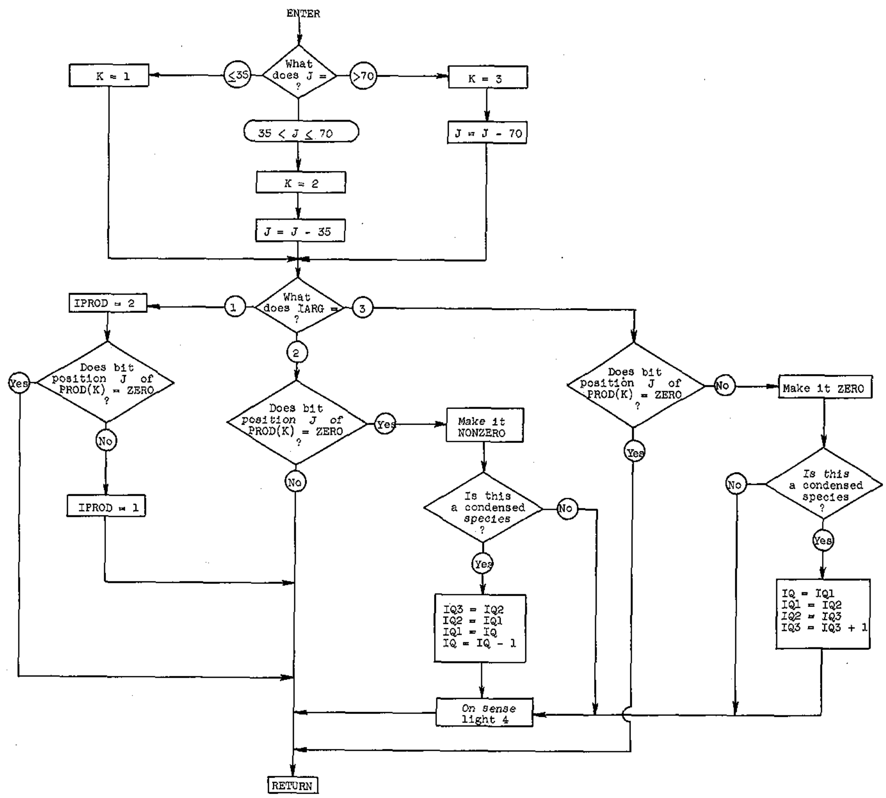


Figure 7. - Subroutine BYPASS.

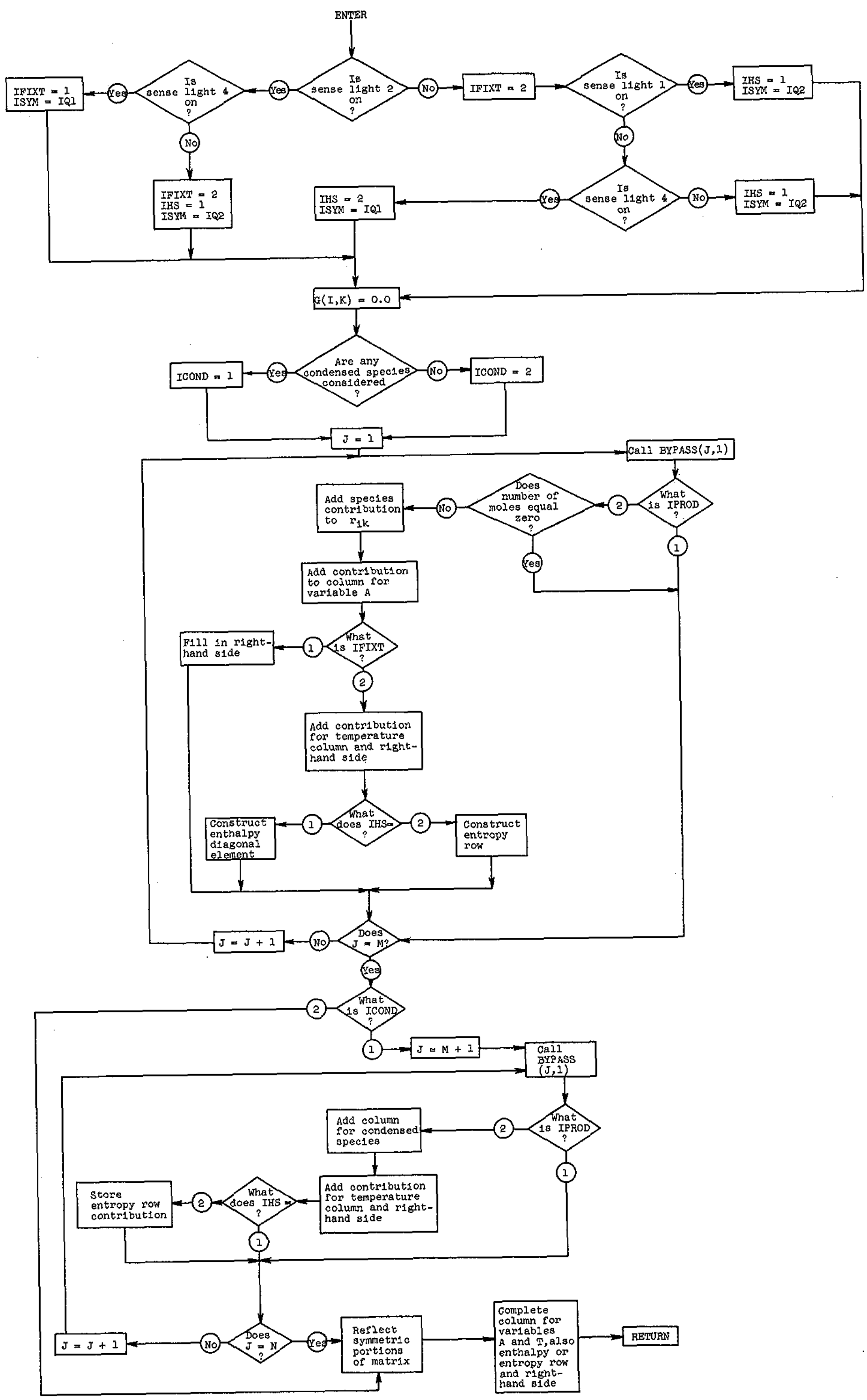


Figure 8. - Subroutine MATRIX.

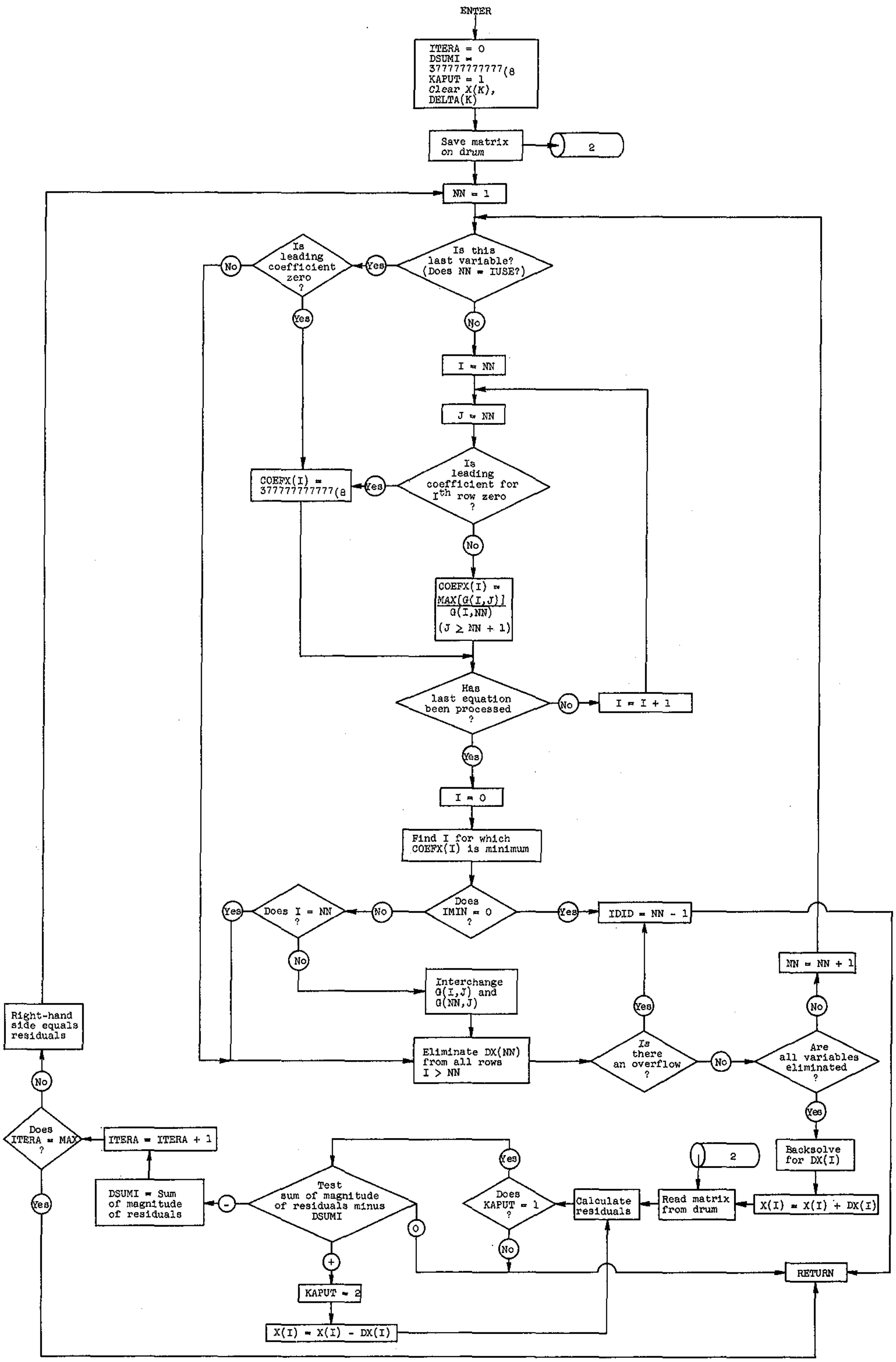


Figure 9. - Subroutine GAUSS.