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FORTRAN IV COMPUTER PROGRAM FOR CALCULATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES OF COMPLEX CHEMICAL SYSTEMS

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16. Abstract

A FORTRAN IV computer program for the calculation of the thermodynamic and transport properties of complex mixtures is described. The program has the capability of performing calculations such as (1) chemical equilibrium for assigned thermodynamic states, (2) theoretical rocket performance for both equilibrium and frozen compositions during expansion, (3) incident and reflected shock properties, and (4) Chapman-Jouguet detonation properties. Condensed species, as well as gaseous species, are considered in the thermodynamic calculations; but only the gaseous species are considered in the transport calculations. Further information on obtaining the program may be had from the authors.

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SUMMARY

A FORTRAN IV computer program for the calculation of the thermodynamic and transport properties of complex mixtures is described. This program (TRAN72) was developed by combining a program for the transport properties calculation with another program (CEC71), published in NASA SP-273, for the thermodynamic properties calculation.

Equations for the calculation of the transport properties are given and explained. Equations for the calculation of the thermodynamic properties can be found in NASA SP-273. Input data, included with the program, are explained.

The program has the capability of performing calculations such as (1) chemical equilibrium for assigned thermodynamic states, (2) theoretical rocket performance for both equilibrium and frozen compositions during expansion, (3) incident and reflected shock properties, and (4) Chapman-Jouguet detonation properties. Condensed species, as well as gaseous species, are considered in the thermodynamic calculations. However, only gaseous species are considered in the transport property calculations.

The program is available for external distribution. Further information on obtaining the program may be had from the authors.

INTRODUCTION

Many processes in existence today involve complex chemical mixtures, frequently at high temperatures. Some of these mixtures result from combustion processes such as occur in automobiles, aircraft, and rockets. Others occur in processing equipment in the chemical, petroleum, and natural-gas industries. Research equipment, such as shock tubes, also involves high-temperature gas mixtures.

The need frequently arises for the thermodynamic and transport properties of these mixtures, particularly for use in heat- and mass-transfer calculations. Usually, the temperatures of the gases involved are quite high, too high for the properties to be measured directly. Consequently, the properties are calculated. As a result, a number of different computer programs have been written for the property calculations. In general, most of the programs now in existence are designed to calculate either the thermodynamic properties or the transport properties, but not both. These programs are not reviewed herein. References 1 to 4 are a starting point for a review of the programs for calculating the thermodynamic properties. Some programs have also been written for calculating the transport properties (refs. 5 to 9); however, each has its limitations. Some of these programs use approximate equations (refs. 5 to 8). One is limited in the choice of the intermolecular potential energy function (ref. 7). Two programs are designed primarily for ionized gases (refs. 8 and 9).

We have developed a computer program which is designed to avoid these limitations. Rigorous equations are used in the transport calculations, and the transport cross sections are not restricted to any specific potential energy form. The program is a general one, capable of handling any chemical system. However, it does not include ionization, although it is capable of handling incipient ionization. Other important features of this program include simplicity of input, storage of all thermodynamic and transport property data on a master tape, and elimination of any need for advance knowledge of which species will be important. The program is a combination of the NASA Lewis Research Center Chemical Equilibrium Calculations Program (ref. 1) with additional routines to do the transport property calculations. The program will handle a variety of problems. It has the capability for doing calculations such as (1) chemical equilibrium for assigned thermodynamic states (T,P), (H,P), (S,P), (T,V), (U,V), or (S,V); (2) theoretical rocket performance for both equilibrium and frozen compositions during expansion; (3) incident and reflected shock properties; and (4) Chapman-Jouguet detonation properties.

The thermodynamic properties which are tabulated include pressure, temperature, density, enthalpy, entropy, molecular weight, $(\partial \ln V/\partial \ln P)_T$, $(\partial \ln V/\partial \ln T)_P$, specific heat at constant pressure, isentropic exponent, sonic velocity, and composition. The calculated transport properties are viscosity and thermal conductivity. Specific heat and thermal conductivity are calculated for both frozen and equilibrium conditions. Prandtl and Lewis numbers are included. Other properties which are characteristic of the type of problem being run are also calculated. (See the sample problems in appendix D.)

The present report does not cover the equations and numerical techniques used for the calculation of the thermodynamic properties. These are given in NASA SP-273 (ref. 1), which discusses the details of the thermodynamic calculations. The present report does give the equations used in the transport calculations, however. These are

covered in the section TRANSPORT PROPERTY EQUATIONS. Sources of the transport data are given in the section SOURCES OF TRANSPORT AND RELAXATION DATA. Symbols are defined in appendix A. Variables, indices, and constants used in the transport subroutines are given in appendix B. A listing of the entire program is shown in appendix C, and sample problems are shown in appendix D. The sample problems were selected to illustrate many of the various capabilities of the program. Flow charts of some routines are included.

COMPUTER PROGRAM

The TRAN72 computer program was written in FORTRAN IV. At the Lewis Research Center it was checked out on an IBM 7094II/7044 Direct Couple System. It has been used to generate both thermodynamic and transport properties of a number of chemical systems for internal use at Lewis.

The source program is available to other organizations. Thermodynamic and transport data are provided with the program. However, these data are updated periodically; as a result, the answers for the sample problems in appendix D may change somewhat from time to time.

Further information on obtaining the program may be had from the authors.

ASSUMPTIONS AND CAPABILITIES

The program is designed to provide both thermodynamic and transport properties for a wide range of scientific and engineering applications and for a range of independent variables. Thermodynamic data for a large number of ideal gases and condensed species are provided with the program for a temperature range of 300 to 5000 K. Transport data are provided over a wider range in many cases. See the section SOURCES OF TRANSPORT AND RELAXATION DATA for the temperature range for each interaction.

The range of applicability of the thermodynamic calculations is approximately described by the limits of applicability of the ideal-gas law. A reduced-state plot of the thermodynamic properties might give the user an idea of the limits of temperature and pressure. The lower limit for temperature in the transport calculations occurs when ternary and higher order molecular collisions become important. This also defines the upper pressure limit for the transport property calculations. The upper limit for temperature occurs when ionization becomes appreciable. However, incipient ionization can be included in the calculations. But, for increasing ionization, higher approximations are needed in the transport calculations (refs. 10 and 11). Additional comments on this may be found in the discussion of the transport property equations. The lower pressure

limit is given by the onset of the free molecular flow regime, which occurs when the mean-free-path length is of the same order of magnitude as the dimensions of the container. Under these conditions the equations for the transport properties are no longer applicable.

In the computation of the thermodynamic properties the NASA Lewis Research Center CEC71 program (ref. 1) is used. The usual equations for the conservation of mass, momentum, and energy are applied (ref. 1, eqs. (93) to (95)) and the ideal-gas law is assumed. The free energy is minimized by using a Newton-Raphson iteration technique. Composition and properties are calculated for equilibrium conditions and, for some situations, for frozen conditions (sometimes called nonreacting). The effects of chemical kinetics, or finite reaction rates, are not included. TRAN72 handles the same types of problems as does CEC71, including normal shock waves, Chapman-Jouguet detonations, rocket expansion problems, and properties at assigned thermodynamic states. The additional assumptions for each type of problem are as follows:

(1) Shock waves are of negligible thickness and normal to the direction of flow. One-dimensional flow is assumed.

(2) For Chapman-Jouguet detonations the Mach number of the wave front, based on the speed of sound in the burned gas, is unity. The assumptions mentioned previously for shock waves also apply.

(3) For rocket combustion problems, it is assumed that there is complete mixing in the chamber, adiabatic combustion at constant pressure, isentropic expansion with complete mixing, and frictionless one-dimensional flow. It is also assumed that the chamber is large enough that the velocity in the chamber is negligible.

Because of storage limitations on the IBM 7094, the maximum allowable number of species is 100 and the maximum number of elements is 10. This applies to the thermodynamic property calculations and includes gases, liquids, and solids. In doing the transport calculations, no more than 20 of the species are used. First the composition obtained from the thermodynamic calculations is searched for the 20 gaseous species with the largest concentrations. However, all gaseous species with mole fractions of less than 10^{-7} are omitted. Then this gaseous composition is normalized by summing the concentrations of these 20 species and dividing each concentration by the sum. The mole fractions obtained by this normalization procedure are the ones used in the transport property calculations.

DESCRIPTION OF PROGRAM INPUT

The procedure for operating the program is relatively simple and is almost identical to that for operating the CEC71 program (ref. 1).

The input specifies the type of problem to be run, the chemical system of interest, the mixture ratio, and the range of variables. Considerable flexibility is available in specifying the variables. For example, in a rocket combustion problem, nozzle expansion points can be specified as pressure ratios, area ratios, or a combination of both. In addition, a number of options are available, such as the following:

(1) The calculated thermodynamic and transport properties may be obtained on punched cards, as well as printed output.

(2) For rocket and shock problems, both equilibrium and frozen properties are available. In particular, for rocket expansion problems, freezing can be made to occur at the chamber, the throat, or any supersonic point in the nozzle. For this type of problem, equilibrium flow is assumed from the chamber to a previously designated station in the nozzle. After that station is reached, the composition is frozen.

(3) Input can be specified in a number of different units. For instance, pressure can be given in mm Hg, atmospheres, psia, or newtons/meter^2.

(4) Species may be omitted from consideration in the calculations through the use of OMIT cards. Also, certain condensed phases may be included in the initial composition through the use of INSERT cards. Otherwise, only gases are considered initially, which may lead to convergence difficulties.

(5) Thermodynamic property calculations can be obtained without including transport property calculations. If this option is used, the program is essentially the same as the CEC71 program. The opposite is not possible. Transport properties cannot be calculated without first doing the thermodynamic property calculations, since the results of the thermodynamic calculations are needed in the transport calculations.

The input data are discussed under four categories. Three of the categories are required and one is optional. The three required categories and the code names by which they are referred to herein are

(1) Library of thermodynamic and transport data for reaction products (THERMO and TRANSPORT data library)

(2) Data pertaining to reactants (REACTANTS cards)

(3) Namelist data, which include the type of problem, required schedules, and options (NAMELISTS input)

The optional category of data is the list of chemical formulas of species which are singled out for special purposes (OMIT and INSERT cards).

Each category of data is discussed in this report. Many of the details are summarized in tables I to VI. Both input and output for 10 sample cases are given in appendix D. These cases are identified by the numbers 51, 52, 122, 123, 679, 950, 1207, 1565, 5612, and 6666. The order of the input is indicated in table II.

THERMO and TRANSPORT Data Library

A library of thermodynamic and transport data is included with each program distributed. The thermodynamic data for reaction products are in the functional form discussed in the section THERMODYNAMIC DATA. The transport data are in a tabular form. The order and format of the THERMO and TRANSPORT data are detailed in table I.

THERMO and TRANSPORT data may be read either from cards or from tape. If the data are read from cards, the program will write these data on logical tape 4. However, a permanent tape or disk containing the data may be made during any run by using the required type of control cards preceding the operating deck. When the data are read from cards, the data are preceded by a code card which has the word THERMO punched in columns 1 to 6. The sample cases in appendix D assume a permanent tape is available. Thus, the THERMO code card and the data are omitted and the input data all start with the REACTANTS cards described in the next section. When data for various species are added, removed, or changed on the tape, the whole set of THERMO and TRANSPORT data cards must be included in the input for making a new tape.

These TRANSPORT data follow immediately after the END card for the THERMO data. No general identification card is needed to indicate the beginning of the TRANSPORT data.

During a computer run, the appropriate reaction-product data consistent with each new set of REACTANTS cards will be automatically selected from the data on tape 4 and stored in core.

REACTANTS Cards

This set of cards is required for all problems. The first card in the set contains the word REACTANTS punched in card columns 1 to 9. The last card in the set is blank. In between the first and last cards may be any number of cards to a maximum of 15, one for each reactant species being considered. The cards for each reactant must give the chemical formula and the relative amount of the reactant. For some problems, enthalpy values are required. The format and contents of the cards are summarized in table III. A list of some REACTANTS cards is given in table IV.

Relative amounts of reactants. - The relative amounts of reactants may be specified in several ways. They may be specified in terms of moles, mole fraction, or mole percent (by keypunching M in card column 53) or in terms of weight, weight fraction, or weight percent (blank in column 53). For example, in appendix E, cases 679 and 1207 specify reactants in terms of moles and case 51 specifies them in terms of weight.

For these cases, the relative amounts of the reactants are completely specified by the values on the REACTANTS cards. However, there are optional variables which may be set in namelist INPT2 that indicate relative amounts of total fuel to total oxidants. (See table V and section NAMELISTS input.) For this situation, each reactant must be specified as a fuel or an oxidizer by keypunching an F or O, respectively, in column 72 of the REACTANTS card. The amounts given on the REACTANTS cards are relative to total fuel or total oxidant rather than to total reactant.

Tables V, VI, and VII describe the namelists. Referring to table V, there are four options in INPT2 for indicating relative amounts of total fuel to total oxidant. They include

(1) Equivalence ratio, r (ERATIO is TRUE)

(2) Oxidant-to-fuel weight ratio, O/F (OF is TRUE)

(3) Fuel percent by weight, %F (FPCT is TRUE)

(4) Fuel-to-air or fuel-to-oxidant weight ratio, F/A (FA is TRUE)

For each option, the values are given in the MIX array of INPT2. This feature is illustrated by cases 52, 122, 950, 5612, and 6666 in appendix D. Cases 52 and 950 show where ERATIO is TRUE (ERATIO = T), and the reactants are identified as fuel or oxidant in card column 72. Since these cases involve just one fuel and one oxidant, the amounts of each (as given in columns 46 to 52) are shown as 100. This means that the oxidizer is 100 percent of the total oxidizers and the fuel is 100 percent of the total fuels. Cases 122 and 5612 are examples which have more than one fuel. Case 122 shows that each fuel is 50 percent (by weight) of the total fuels and the one oxidizer is 100 percent of the total oxidizer.

The purpose of the previous namelist variables is to permit using one set of reactant cards with any number of values (maximum, 15) of a variable. Case 950, for example, specifies three values of equivalence ratio (ERATIO = T).

Reactant enthalpy. - Assigned enthalpy values for initial conditions are required for assigned enthalpy and pressure (HP), rocket (RKT), detonation (DETN), and shock (SHOCK) problems. An assigned internal energy is required for the assigned internal energy and volume (UV) problem. These assigned values for the total reactant are calculated automatically by the program from the enthalpies or internal energies of the individual reactants. The enthalpy values for the individual reactants are either keypunched on the REACTANTS cards or calculated from the THERMO data. The choice varies according to the type of problem as follows:

(1) RKT, UV, and HP problems: Enthalpies or internal energies are taken from the REACTANTS cards unless zeros are punched in card columns 37 and 38. For each REACTANTS card with the "00" code, an enthalpy will be calculated for the species from the THERMO data for the temperature given in card columns 64 to 71. See MgO(s) in case 51, appendix D.

(2) SHOCK problems: Enthalpies for all the reactants are calculated from the THERMO data for the temperatures in the T schedule of namelist INPT2 (table V). If enthalpy values are punched in card columns 64 to 71 (table III), they will be ignored. It is not necessary to punch zeros in card columns 37 and 38.

(3) DETN problems: If no T schedule is given in namelist INPT2, the option for calculating reactant enthalpies is the same as for RKT, UV, and HP problems. However, if a T schedule is given in INPT2, the enthalpies will be calculated from the THERMO data for the temperatures in the T schedule, the same as for the SHOCK problem.

When the program is calculating the individual reactant enthalpy or internal energy values from the THERMO data, the following two conditions are required:

(1) The reactant must also be one of the species in the set of THERMO data. For example, $NH_3(g)$ is in the set of THERMO data but $NH_3(\ell)$ is not. Therefore, if $NH_3(g)$ is used as a reactant, its enthalpy could be calculated automatically but that of $NH_3(\ell)$ could not be.

(2) The temperature T must be in the range $T_{low}/1.2 \leq T \leq T_{high} \times 1.2$, where T_{low} to T_{high} is the temperature range of the THERMO data.

NAMELISTS Input

As indicated in table II, the NAMELISTS code card precedes the NAMELISTS input. The card has the word NAMELISTS punched in card columns 1 to 9. All problems require an INPT2 input. Rocket and shock problems each require an additional set, namely RKTINP or SHKINP. The additional set simply follows INPT2 directly.

The variables in each namelist are listed in tables II, V, VI, and VII. Table II indicates which variables are required and which are optional for the various types of problems. Tables V, VI, and VII give a brief definition of each variable. Some additional information about some of these variables follows:

Pressure units. - The program assumes the pressure in the P schedule to be in units of atmospheres unless either PSIA = T, NSQM = T, or MMHG = T.

Relative amounts of fuel (or fuels) and oxidizer (or oxidizers). - These quantities may be specified by assigning 1 to 15 values for either O/F, %F, F/A, or r. If no value is assigned for any of these options, the program assumes the relative amounts of fuel (or fuels) and oxidizer (or oxidizers) to be those specified on the REACTANTS cards. (See discussion in section REACTANTS Cards.)

Printing mole fractions of trace species. - The program normally prints only the compositions of those species with mole fractions greater than 5×10^{-6} in F-format for all problems except SHOCK. The TRACE option permits printing smaller mole fractions. If the variable TRACE is set to some positive value, mole fractions greater than or equal

to this value will be printed. When this option is used, a special E-format for mole fraction output is used automatically. A TRACE value of 1.E-38 is the lowest value allowed by the program. (See case 1565 in appendix E.)

For SHOCK problems, mole fractions of trace species are often desired. Thus, for SHOCK problems, the program will set TRACE to 5.E-9 automatically, and the E-format for output is always used. This value may be changed by using the TRACE option in INPT2 namelist input. (See case 1207 in appendix E.)

TP, HP, SP, TV, UV, or SV problems. - In these problems, from 1 to 52 values of T, and from 1 to 26 values of P or V (or RHO) may be assigned. However, only one value of entropy S0 may be assigned in INPT2 for the SP or SV problem. Only one value of enthalpy is permitted for the HP problem, and only one value of internal energy is permitted for the UV problem. However, these values of enthalpy and internal energy are not assigned in INPT2 but are calculated by the program. In a TP problem, if 52 values of T and 26 values of P are assigned in INPT2, properties will be calculated for the 1352 possible P and T combinations. Similarly, as many as 1352 combinations can be calculated for a TV problem.

DETN problem. - Calculations will be made for all combinations of initial pressure P and initial temperature T. Initial temperatures may be specified in INPT2 namelist or on the REACTANTS card.

RKT problem. - At least one chamber pressure value P is required in INPT2, although as many as 26 chamber pressures may be assigned. A complete set of calculations will be made for each chamber pressure. The RKT problem requires a second namelist for input, RKTINP, which is discussed in the next section.

RKTINP namelist (RKT problem only). - This namelist is required for RKT problems. It follows the INPT2 namelist. A list of variables and definitions is given in table VI. Even though this namelist is required, all variables are optional. If no variables are assigned, only the chamber and throat conditions will be calculated. Usually, a pressure ratio schedule (PCP), an area ratio schedule (SUBAR or SUPAR), or some combination of these schedules will be assigned.

Pressure ratio and area ratio schedules must not include values for the chamber and throat, inasmuch as these values are calculated automatically by the program. If both a pressure ratio schedule and an area ratio schedule are given in RKTINP, the pressure ratios will be calculated first. If both schedules are omitted, only chamber and throat conditions will be calculated.

The program will calculate both equilibrium and frozen performance, unless RKTINP has the logical variable FROZ set equal to FALSE (FROZ = F) or the logical variable EQL set equal to FALSE (EQL = F). If FROZ = F, only equilibrium performance will be calculated. If EQL = F, only frozen performance will be calculated.

If a frozen expansion is being calculated, it is possible to specify the freezing point by using the variable NFZ. For instance, to freeze immediately after the fifth point, set

NFZ = 5. If NFZ is not specified in the RKTINP namelist, the program assigns NFZ = 1 (freezing in the chamber). If NFZ = 1 or 2 (NFZ = 2 corresponds to the throat), 22 additional stations may be assigned in the expansion. If NFZ > 2, the program will allow only 11 additional stations. Freezing is permitted in the chamber, the throat, or any supersonic station but not at a subsonic station.

SHOCK problem. - The program requires a P and T schedule in INPT2, and a schedule of either initial velocities (U1) or Mach numbers (MACH1) in a second namelist, SHKINP (see table VII). These values of P, T, and either U1 or MACH1 all refer to the unshocked gas and must correspond one-to-one with each other. Case 1207 in appendix D is a shock problem. The pressure and temperature schedules are limited to 13 values for SHOCK problems only. This corresponds to the 13-value limit for U1 or MACH1 schedules.

REACTANTS cards must be only for gaseous reactants that are also included as reaction species in the THERMO data. This permits the program to calculate enthalpy and specific-heat values of the reactants from the THERMO data.

SHKINP namelist (SHOCK problem only). - A list of variables and definitions is given in table VII. SHKINP must include from one to 13 values of either U1 or MACH1 of the unshocked gas. The program will calculate incident shock parameters that assume both equilibrium and frozen composition unless SHKINP has the logical variable INCDEQ set equal to FALSE (INCDEQ = F) or the logical variable INCDFZ set equal to FALSE (INCDFZ = F). If INCDEQ = F, only frozen composition will be used. If INCDFZ = F, only equilibrium composition will be used. In addition, there are options for calculating reflected shock parameters. For each incident condition called for, reflected shock parameters will be calculated that assume either a frozen composition (REFLFZ = T), an equilibrium composition (REFLEQ = T), or both (REFLFZ = T, REFLEQ = T).

OMIT and INSERT Cards

As indicated in table II, OMIT and/or INSERT cards may follow the REACTANTS cards. Their inclusion is optional. They contain the names of particular species in the library of thermodynamic data for the specific purposes to be discussed. Each card contains the word OMIT (in card columns 1 to 4) or INSERT (in card columns 1 to 6) and the names of from one to four species starting in columns 16, 31, 46, and 61. The names must be exactly the same as they appear in the first 12 columns of the THERMO data cards (see table I).

OMIT cards. - Occasionally, it may be desired to specifically omit one or more species from consideration as possible species. This omission may be accomplished by means of OMIT cards containing these species names. See appendix D, cases 51 and 950.

If OMIT cards are not used, the program will consider as possible species all those species in the THERMO data which are consistent with the chemical system being considered.

INSERT cards. - These cards contain the names of condensed species only. They have been included as options for the following two reasons:

The first and more important reason for including the INSERT card option is that, in rare instances, it is impossible to obtain convergence for assigned enthalpy problems (HP or RKT) without the use of an INSERT card. This occurs because the temperature sometimes becomes extremely low (several kelvin) when only gases are considered. In these rare cases, the use of an INSERT card containing the name of the required condensed species will eliminate this kind of convergence difficulty. When this difficulty occurs, the following message is printed by the program: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD."

The second and less important reason is for efficiency of computation. If it is known that certain condensed species will be present among the final equilibrium compositions for the first assigned point, a small amount of computer time can be saved by using an INSERT card. The inserted condensed species will then be considered by the program during the initial iterations for the first assigned point. If the INSERT card were not used, only gaseous species would be considered during the initial iterations. However, after convergence, the program would automatically insert the appropriate condensed species and reconverge. For all other assigned points the inclusion of condensed species is handled automatically by the program. Therefore, it usually is immaterial whether or not INSERT cards are used for the purpose of saving computer time.

DESCRIPTION OF PROGRAM OUTPUT

The program prints four kinds of output: input data used to do the calculations, information concerning iteration convergence, tables of results, and optional intermediate output.

Input Data

Input data have been previously described. The general procedure used in this program is to list the input as they are read in and before they are processed by the program. The purpose is to show, in as clear a way as possible, what is actually on the input cards. All problems list the following input data:

(1) The word REACTANTS

(2) Reactant data

(3) INSERT and/or OMIT card data

(4) The word NAMELISTS

(5) All data in namelist INPT2 given in table V (P and RHO use same storage)

Following the INPT2 data is the statement "SPECIES BEING CONSIDERED IN THIS SYSTEM." Each species in the list is preceded by some identification, such as J12/65. The J refers to JANAF data (JANAF Thermochemical Tables, see ref. 1). The letter L refers to unpublished data calculated at the Lewis Research Center. The number refers to the month and the year the data were published or calculated (12/65 is December 1965).

For a rocket problem, the namelist RKTINP data given in table VI are listed. For a shock problem, the namelist SHKINP data given in table VII are listed.

Following the list of chemical species (or RKTINP or SHKINP data, if any) is the current value of O/F. This is followed by a listing of the enthalpies or internal energies of the total fuel and oxidant and of the total reactant. Following this is a list of the kilogram-atom per kilogram of each element in the total fuel and oxidant in the total reactant.

Tables of Thermodynamic Results

The final output of the program is in the form of tables that are designed to be self-explanatory. Tabulated properties include pressure P, temperature T, density ρ, enthalpy h, entropy s, molecular weight M, two partial derivatives $(\partial \ln V/\partial \ln P)_T$ and $(\partial \ln V/\partial \ln T)_P$, specific heat c_p, isentropic exponent γ_S, and velocity of sound a. (An option is available to punch these values on cards. See table V and case 123 in appendix D.) Compositions are also included and given in terms of mole fractions. In addition, rocket, shock, and detonation problems each list additional calculated properties which are pertinent to each type of problem.

Tables of Transport Results

The printed output consists of calculated results in tabular form. Punched-card output is also available as an option. With the exception of the heading at the top, the output for the transport calculations is the same for all types of problems. Viscosities, thermal conductivities, specific heats, Prandtl numbers, and Lewis numbers are calculated and listed for the same conditions as shown in the results of the thermodynamic calculations.

Both frozen and equilibrium values are shown for the thermal conductivity, specific heat, and Prandtl number. The difference between frozen and equilibrium can be described in the following way: Consider a system of reactive species initially in chemical

equilibrium. If heat is then either added or removed, the temperature and pressure will change. If the composition does not change from the initial state, the system is said to be frozen. If the composition adjusts to the equilibrium composition of the new temperature and pressure, the system is said to be in equilibrium. But, if the final composition is neither of these two conditions, the effects of chemical kinetics must be considered. As stated previously, however, the effects of chemical kinetics are not included in the program.

The specific heats shown in the transport properties table are usually identical with those shown in the thermodynamic properties table. However, differences do frequently occur for perfectly valid reasons. These are explained in the section TRANSPORT PROPERTY EQUATIONS.

At this point it is worth explaining why the calculation of the specific heat is repeated in the transport property calculations, with condensed phases omitted. The reason is that it enables the calculation of internally consistent Prandtl and Lewis numbers, numbers derived from properties which are all based on the same gaseous composition. These may be preferable for use in heat- and mass-transfer calculations.

Error Messages

The only other printed output which can occur comes from any one of a number of programmed error messages. Most of these are in the subroutines which do the thermodynamic property calculations. These are explained in detail in reference 1. Four programmed error messages occur in the transport property subroutines. Two are in subroutine TRANSP and the other two are in subroutine INPUT. These messages are explained in the sections discussing the subroutines.

THERMODYNAMIC DATA

Thermodynamic data are included with the program. Reference 1 lists data for 62 reactants and 421 reaction species (solid, liquid, and gas phases of a species are counted as separate species).

Assigned Enthalpies

For each species, heats of formation (and, when applicable, heats of transition) were combined with sensible heats to give assigned enthalpies H_T^o. By definition,

$$H_T^o \equiv H_{298.15}^o + \left(H_T^o - H_{298.15}^o\right) \quad (1)$$

We have arbitrarily assumed $H_{298.15}^o = \left(\Delta H_f^o\right)_{298.15}$. Equation (1) then becomes

$$H_T^o = \left(\Delta H_f^o\right)_{298.15} + \left(H_T^o - H_{298.15}^o\right) \quad (2)$$

In general, $H_T^o \neq \left(\Delta H_f^o\right)_T$ for $T \neq 298.15$ K. For reference elements, $\left(\Delta H_f^o\right)_{298.15} = H_{298.15}^o = 0$. For the species included with the program these reference elements are Al(s), Ar(g), B(s) (beta), Be(s), $Br_2(l)$, C(s) (graphite), Cl_2(g), Cs(s), F_2(g), Fe(s), H_2(g), He(g), K(s), Li(s), Mg(s), N_2(g), Na(s), Ne(g), O_2(g), P(s) (red, V), S(s) (rhombic), Si(s), and Xe(g).

Assigned enthalpies for reactants are given in table IV (in cal/mole as required for program input) together with some other reactant data. For cryogenic liquids, assigned enthalpies are given at their boiling points. These are usually obtained by subtracting the following quantities from the heat of formation of the gas phase at 298.15 K: sensible heat between 298.15 K and the boiling point, difference in enthalpy between ideal gas and real gas at the boiling point, and heat of vaporization at the boiling point.

Least Squares Coefficients

For each reaction species, the thermodynamic functions specific heat, enthalpy, and entropy as functions of temperature are given in the form of least squares coefficients as follows:

$$\frac{C_p^o}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \quad (3)$$

$$\frac{H_T^o}{RT} = a_1 + \frac{a_2}{2}T + \frac{a_3}{3}T^2 + \frac{a_4}{4}T^3 + \frac{a_5}{5}T^4 + \frac{a_6}{T} \quad (4)$$

$$\frac{S_T^o}{R} = a_1 \ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7 \quad (5)$$

Reference 12 describes a program which calculates the thermodynamic functions and fits the functions to equations of the form given in equations (3) to (5).

TRANSPORT DATA

Transport and relaxation data are provided for 59 species, and additional transport data are provided for interactions between unlike species for another 58 interactions. Sources of these data are described in the section SOURCES OF TRANSPORT AND RELAXATION DATA and in tables VIII and IX. All data are in tabular form as a function of temperature. In contrast with the thermodynamic data, the temperature range of the transport data is not the same for all interactions. The temperature ranges for the transport data are also shown in table VIII.

The temperature intervals in the table are not constant, but generally increase with increasing temperature. This was done in order to accommodate interpolation within the table. Interpolation is done by four-point Lagrange, and the number of arguments allowed per table is 20. This number was arrived at as a compromise between two considerations. First, storage space is limited (IBM 7094); and in order to allow sufficient storage for a large number of interactions, the number of intervals in each table should not be excessive. However, the interval size must be small enough such that interpolation errors are less than the uncertainty of the data within the table. Consequently, the temperature intervals tend to be closest in the vicinity of 300 K because usually the transport data are most accurately known at room temperature.

SAMPLE PROBLEMS

Ten sample problems are given to illustrate some of the features of the program. Five are rocket performance problems, RKT = T (cases 51, 122, 679, 5612, and 6666); two are combustion problems (case 123 is for combustion at constant pressure, HP = T; and case 1565 is for combustion at constant volume, UV = T); case 52 is a detonation problem, DETN = T; case 1207 is a shock problem, SHOCK = T; case 950 is an assigned temperature and pressure problem, TP = T; and case 6666 illustrates freezing in a rocket at a location other than the chamber.

It would not be practical to illustrate every possible combination of options permitted by the program. However, the sample problems were selected to illustrate many of the possible combinations and, in particular, those variations which we believe would most often be used. Included in the combinations illustrated are the following:

(1) Specifying proportions of various reactants
   (a) O/F: cases 122, 123, and 1565
   (b) Equivalence ratios: cases 52 and 950
   (c) Percent fuel by weight: cases 5612 and 6666
   (d) Complete information on reactant cards: cases 51, 679, and 1207

(e) Relative weights of reactants: cases 51, 52, 122, 123, 950, 1565, 5612, and 6666

(f) Relative moles of reactants: cases 679 and 1207

(2) Specifying enthalpies

(a) On reactant cards: cases 51 (partly), 122, 123, 679, 950, 1565 (partly), 5612, and 6666

(b) Calculated by program: cases 51 (partly), 52, 1207, and 1565 (partly)

(3) Pressure units

(a) psia: cases 51, 122, 679, 5612, and 6666

(b) atm: cases 52, 123, and 950

(c) mm Hg: case 1207

(4) INSERT: cases 51 and 5612

(5) OMIT: cases 51 and 950

(6) Composition in floating-point format: case 1565

(7) Program considers ions: case 679

(8) Special derivatives due to two condensed phases of a species: cases 51 and 5612

(9) Special throat interpolation: case 5612

(10) Omit transport property calculations: case 679

(11) Punched-card output: case 123

(12) Freezing at supersonic station: case 6666

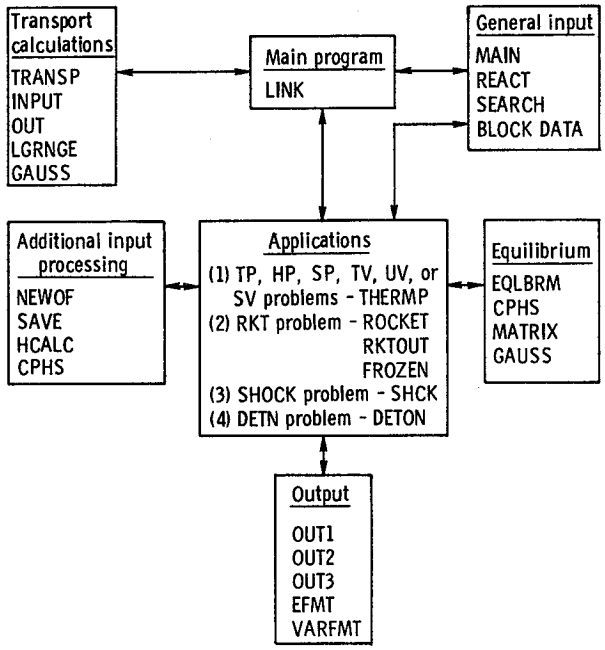
Some additional features of the program illustrated by the various cases are the following:

(1) Case 51: This case shows several condensed species being automatically inserted and removed by the program. Frozen expansion is stopped at point 3 inasmuch as the exit temperature is below the melting point of 2315 K.

(2) Case 122: This case shows that it is possible to assign a schedule of points which includes a mixture of pressure ratios, subsonic area ratios, and supersonic area ratios.

MODULAR FORM OF PROGRAM

In order to facilitate adding or deleting applications of the chemical equilibrium part of the program, the program was set up in 10 modules. These modules are concerned with overlay control, which is used on the IBM 7094 (main program), and with general input, additional input processing, four applications, equilibrium calculations, transport calculations, and output. The general flow of these modules and associated routines is given in the following schematic:



From this diagram, it is clear that, for example, the rocket application could be eliminated by omitting subroutines ROCKET, RKTOUT, and FROZEN and by omitting the statement which calls ROCKET in the main program.

LINK (MAIN PROGRAM)

LINK is the main program. Its sole function is to control the program flow between the thermodynamic and transport property calculations. The overlay structure used for the IBM 7094 is shown in figure 1. LINK and subroutine GAUSS are the only two routines in core storage at all times. (GAUSS solves a set of as many as 20 simultaneous linear equations.) Overlay is not required for machines which have sufficient storage for the entire program.

A flow chart of LINK is given in figure 2.

The number of storage locations used for each routine is shown in parentheses in figure 1. These numbers include allocations for block common, as they are introduced into storage in loading the program. That is, the number in parentheses includes a block common with the first routine in which it is used. Consequently, LINK and TRANSP have larger numbers than they would have if the common blocks had not been included.

When the program is doing thermodynamic property calculations, LINK 0 and LINK 1 are in core storage. This uses about 27 000 storage locations. When the program is doing transport property calculations, LINK 0 and LINK 2 are in core storage. This uses over 32 000 storage locations. These numbers include all the routines but not other storage needed by the computer system. This additional storage requirement will vary from

one computer installation to another. At NASA Lewis this amounts to 1548 storage locations for the system and an additional 5590 for the systems subroutines, for a total of 7138 additional storages.

DISCUSSION OF SUBROUTINES

This section describes the routines not included in reference 1 and also describes those in the CEC71 program which have been changed. Among the new routines are the subroutines needed for the transport property calculations and the main program (LINK), which links the thermodynamic calculations with the transport calculations. Subroutines which will not be discussed are those which are nearly the same as those in reference 1.

Some dimensions have been changed from the CEC71 program. In order to save storage, only 100 species and 10 elements are permitted, rather than 150 species and 15 elements, as are allowed in CEC71. Also, the number of temperatures T has been changed from 26 to 52. These dimension changes apply to any routine in which the variables appear. These changes affect the common blocks POINTS, SPECES, and MISC.

Two new common blocks, SAVED and CONTRL, have been added. SAVED is used to save information obtained from the thermodynamic calculations which is needed in the transport calculations. It is also used to save information obtained from the transport calculations which is needed later. This change also caused a slight reorganization of the variables in common blocks SPECES, MISC, and INDX. CONTRL contains additional logical variables TRNSPT, FROZN, PUNCH, and NODATA.

Flow charts are also included for aid in understanding of the program. The reader may find appendixes A and B helpful in relating symbols to the program variable names.

Subroutine MAIN

Subroutine MAIN is very similar to the main routine in the CEC71 program. A flow chart is given in figure 3. Perhaps the most noteworthy change is that it is now a subroutine. One other change is significant. That is, when thermodynamic data are being read in from cards, transport and relaxation data immediately follow the thermodynamic data. The format for the thermodynamic data is still the same as in reference 1. This change essentially involves only the insertion of 11 additional cards which are needed in order to read and write the transport and relaxation data on tape unit 4.

Subroutine SEARCH

SEARCH searches for data stored on logical tape unit 4. Thermodynamic data for all the species in the chemical system are located on tape unit 4 and saved in core storage. In addition, transport and relaxation data are also read from tape unit 4, and the data which are relevant to the chemical system are stored on logical tape unit 3 (disk storage).

Another search of the transport and relaxation data on tape unit 3 is made at the start of the transport property calculations in subroutine TRANSP. This second search is used in order to find the data involving interactions of only the important species and to save these data in core storage. This secondary search is discussed in the section Subroutine TRANSP.

Subroutine OUT1

Subroutine OUT1 is the output routine for the thermodynamic calculations. It is nearly the same as OUT1 in the CEC71 program. The only change is that punched-card output of the thermodynamic properties is now included. Only data of the standard thermodynamic properties which apply to all types of problems (rocket, shock, detonation, and assigned thermodynamic states) are punched. The additional properties, which apply only to the particular type of problem being run, are not punched.

Subroutines THERMP, ROCKET, SHCK, and DETON

These subroutines control the calculations for the same types of problems as in the CEC71 program: properties at assigned thermodynamic states, rocket combustion, normal shock waves, and Chapman-Jouguet detonations. The basic differences between the two programs are the modes of entry and return from these routines. Both standard and nonstandard entries and returns are used, in contrast with the CEC71 program, which uses only a standard entry and return. The modes of entry and return can be seen from figure 2 and the program listing (appendix C).

Another difference between the programs involves the DO loops on pressure, temperature, and O/F (P, T, OXF). The subroutines for the thermodynamic calculations and the subroutines for the transport calculations are in different core loads. So if the problem involves more than 13 points, the core load for the thermodynamic calculations has to be reloaded after each set of transport calculations is completed. However, in order to reenter the subroutines THERMP, ROCKET, SHCK, and DETON after each set of transport calculations, it would have been necessary to illegally enter inside the DO

loops. To avoid this problem, the DO loops have been eliminated and a simple, program-generated, indexing procedure on P, T, and OXF has been used.

Subroutine ROCKET has additional changes associated with the variable NFZ, the variable which specifies the freezing point for frozen flow. Since the CEC71 program permits only freezing at the chamber, the present program required some changes in order to allow freezing at the throat or at any supersonic station.

Subroutine TRANSP

Subroutine TRANSP is the main routine for the transport calculations. A flow diagram is given in figure 4. All calculations of the properties are done in this routine. The equations are given in the next section.

One other operation is carried out in this routine. Logical tape unit 3 is searched for the transport and relaxation data of the important interactions and saved in the variable TABLES. This search differs from the one in subroutine SEARCH. In SEARCH, data are saved for all interactions in the chemical system; whereas, in TRANSP, interactions involving a trace species are eliminated.

The remainder of the routine is the calculation of the properties. Calculation of the viscosity, monatomic thermal conductivity, reaction thermal conductivity, and reaction heat capacity all involve the solving of a set of simultaneous linear equations. The matrix elements for each are calculated in TRANSP, but the actual solution is obtained from subroutine GAUSS.

The solutions obtained from GAUSS are checked for accuracy for two of the properties, viscosity and reaction thermal conductivity. If the initial equations are not satisfied to a prescribed tolerance by using the solution obtained from GAUSS, an error message is printed out. (See the listing in appendix C of subroutine TRANSP for the specific information printed out in each error message.)

Subroutine INPUT

Subroutine INPUT sets up the transport and relaxation data needed for the transport property calculations done in TRANSP. It is called from TRANSP for each point. The various functions of this subroutine are outlined as follows:

(1) The EN array is searched for the most important gaseous species for the current point. These are identified and saved by storing the index of the species name in IND. A maximum of 20 species is allowed. All species of mole fractions less than 10^{-7} are omitted, as well as all condensed phases. However, all gaseous atomic elements are initially included, even if they are not among the 20 most important species, or even if

their mole fractions are less than 10^{-7}. This condition is imposed to satisfy a requirement imposed upon the A array, which is explained later in this section. If any elements have been omitted through use of an OMIT card, they are reinserted into the A array at this point. A message is printed out giving the name of the element reinserted into the A array: "NO ELEMENT WAS FOUND IN THE LIST OF SPECIES WITH THE NAME (name of species), OR ELSE THERE IS AN ERROR IN THE A(I,K) ARRAY."

(2) The mole fractions and molecular weights are now calculated for the new reduced composition obtained in step 1.

(3) Transport and relaxation data are initialized to zero. Then, data stored in TABLES are searched, interaction by interaction, for data pertinent to the current point. When such data are found, subroutine LGRNGE(TT) is called. LGRNGE(TT) interpolates for the temperature TT. If data are missing for a pure species, an empirical equation is used to estimate the data. If data are missing for an interaction between unlike species, data are estimated from combining rules, using the data of the pure species. The empirical equation and the combining rules are described in the next section. If data for a pure species are missing, an error message is printed out: "NO TRANSPORT DATA WERE FOUND FOR THE SPECIES (name of species)." If the logical variable NODATA is not specified in the INPT2 namelist, the program sets NODATA = .F. and the message is printed. If NODATA = .T. is set in namelist INPT2, the message is not printed. However, no message is ever printed when data are missing for an interaction between unlike species. In either case, the program continues.

The purpose of this error message is to warn the program user when transport data for a major species are missing. When the user is certain this is not the situation, he may wish to omit the message, in order to avoid getting the message every time the program fails to find data for a minor species.

(4) The final operation of INPUT is to read the stoichiometric coefficients from the A array into the STC array and reorder them so as to express them as a set of chemical reaction equations, suitable for use in equation (25). As was mentioned earlier, all the elements in the system are initially included. This is not a necessary requirement, but was done as a matter of convenience. By including all the elements among the 20 (or less) gaseous species in the system, it is possible to use the A array to express the system in terms of a sufficient set of independent chemical equations. The number of required independent equations is given by taking the total number of species and subtracting the number of chemical elements in the system. So by choosing the set of chemical equations as the chemical reactions of formation of each species, a set of equations can be easily written directly from the stoichiometric coefficients in the A array. For instance, in the A array corresponding to the column for CH_4, there is a 1 in the row for carbon, a 4 in the row for hydrogen, and a 0 in the rows for the remaining elements. By assigning a -1 to CH_4, the chemical equation $C + 4H - CH_4 = 0$ is formed.

This procedure is applied to each species in the system, and the result is the initial set of equations. This initial set of equations is then reduced in order to eliminate any species or element (in this case always an element) not found among the 20 most important species in the system. This reduction is accomplished by searching through the chemical equations for an element with a mole fraction less than 10^{-7}, solving the chemical equation for that element, and then substituting the result in any other equation in which the element appears. The new set of equations is one less in number than the original set. This procedure is repeated until all the elements of mole fractions less than 10^{-7} have been eliminated from the chemical equations. The stoichiometric coefficients of this final set of equations are stored in STC and are used in equation (25) for calculating the reaction contribution to the heat capacity and thermal conductivity.

Subroutine OUT

The output routine, appropriately called OUT, handles all the output of the transport property calculations. This includes table headings, units, calculated data, spacing, and punched-card output.

This routine was written with the capability of saving the transport data for as many as 52 points. These data are saved in STORE. Including the current set of 13 points, this means that as many as 65 points can be printed at one time. If the problem has more than 65 points, such as might occur for a TP problem, transport data will be printed out after every multiple of 65 points.

Subroutine LGRNGE(TT)

Subroutine LGRNGE(TT) is a four-point Lagrange interpolation routine. It is used to interpolate within the tables of transport and relaxation data at temperature TT.

TRANSPORT PROPERTY EQUATIONS

The rigorous theory for the transport properties of real, dilute, monatomic gases has been reviewed and studied in great detail by Chapman and Cowling (ref. 13) and Hirschfelder, Curtiss, and Bird (ref. 14). Both references 13 and 14 express the transport coefficients in terms of Sonine polynomial expansions. However, in actually solving the equations, they use different but equivalent methods. Another method originated by Maxwell and refined by Chapman is called the moment method. More recently, Grad (ref. 15) has made the expansion in the moment method more systematic, using Hermite

polynomials rather than Sonine polynomials; his method is frequently referred to as the "thirteen-moment method." An historical review of the early work in this field is given in reference 13.

The methods described in references 13 to 15 result in mathematical solutions with increasing orders of approximation to the transport coefficients. As the order of approximation increases, so does the arithmetic complexity. Fortunately, what is usually referred to as the first approximation is sufficiently accurate for nearly all practical applications. The most notable exception to this is when ionization becomes appreciable (refs. 10 and 11). This is particularly true for the thermal conductivity. The present program uses only the first approximations, and this suggests an upper limit to the range of applicability for the transport coefficient calculations. This limit is incipient ionization. When the degree of ionization is low, collisions between ionized species and neutral particles are infrequent, and collisions where both species are ionized are very infrequent. With a further increase in temperature (or decrease in pressure), ionization increases and interactions between charged particles become important. At this point the first approximation is no longer sufficient.

However, it should be reiterated that what we are referring to here are approximations to the solution of the general equation. There are other assumptions in the mathematical formulation which have been discussed in the section ASSUMPTIONS AND CAPABILITIES. These assumptions restrict the range of applicability of the general equation at high pressures and at low temperatures and pressures.

Viscosity

The viscosity of the gas mixture is calculated from the following equation (ref. 14, p. 489, eqs. (7.4-56) and (7.4-57), see also pp. 531 and 532):

$$\eta_{mixture} = \sum_{i=1}^{n} x_i \eta_i \tag{6}$$

where n is the number of species in the mixture, x_i is the mole fraction of species i, and η_i is found by solving the following set of simultaneous algebraic equations, which are linear in the unknown η_j:

$$\sum_{j=1}^{n} c_{ij} \eta_j = x_i \qquad i = 1, 2, \ldots, n \tag{7}$$

and the c_{ij} matrix coefficients are given by

$$c_{ii} = \frac{x_i^2}{\eta_{ii}} + \sum_{\substack{k=1 \\ k \neq i}}^{n} \frac{2x_i x_k}{\eta_{ik}} \frac{M_i M_k}{(M_i + M_k)^2} \left(\frac{5}{3A_{ik}^*} + \frac{M_k}{M_i} \right) \tag{7a}$$

$$c_{ij} = -\frac{2x_i x_j}{\eta_{ij}} \frac{M_i M_j}{(M_i + M_j)^2} \left(\frac{5}{3A_{ij}^*} - 1 \right) \qquad i \neq j \tag{7b}$$

where

$$\eta_{ij} = \frac{5}{16N_A} \frac{\sqrt{2\pi M_i M_j RT/(M_i + M_j)}}{\pi \bar{\Omega}_{ij}^{(2,2)}} \tag{7c}$$

and

$$A_{ij}^* = \frac{\bar{\Omega}_{ij}^{(2,2)}}{\bar{\Omega}_{ij}^{(1,1)}} \tag{7d}$$

where N_A is Avogadro's number, M_i is the molecular weight of species i, R is the gas constant, T is the temperature, and $\bar{\Omega}_{ij}^{(1,1)}$ and $\bar{\Omega}_{ij}^{(2,2)}$ are cross sections. The $\bar{\Omega}_{ij}^{(1,1)}$ are the diffusion cross sections. When j = i, the $\bar{\Omega}_{ij}^{(2,2)}$ are viscosity cross sections, and η_{ij} simplifies to the equation for the viscosity of a pure gas $\left(5\sqrt{\pi M_i RT}/16\pi N_A \bar{\Omega}_{ii}^{(2,2)}\right)$.

Thermal Conductivity

The thermal conductivity is usually expressed as

$$\lambda_{mixture} = \lambda_{trans} + \lambda_{int} + \lambda_{reaction} = \lambda_{frozen} + \lambda_{reaction} \tag{8}$$

An equation for the first term on the right side of equation (8) was derived by Muckenfuss and Curtiss (ref. 16) and may be written in the form

$$\lambda_{trans} = 4\sum_{i=1}^{n} x_i\lambda_i \tag{9}$$

where the λ_i are found by solving the following set of simultaneous linear equations, similar to those for the viscosity:

$$\sum_{j=1}^{n} b_{ij}\lambda_j = x_i \qquad i = 1, 2, \ldots, n \tag{10}$$

and the b_{ij} matrix coefficients are given by

$$b_{ii} = \frac{4x_i^2}{\lambda_{ii}} + \sum_{\substack{k=1 \\ k\neq i}}^{n} \frac{2x_i x_k \left(\frac{15}{2} M_i^2 + \frac{25}{4} M_k^2 - 3B_{ik}^* M_k^2 + 4A_{ik}^* M_i M_k\right)}{\left(M_i + M_k\right)^2 A_{ik}^* \lambda_{ik}} \tag{10a}$$

$$b_{ij} = -\frac{2x_i x_j M_i M_j}{\left(M_i + M_j\right)^2 A_{ij}^* \lambda_{ij}} \left(\frac{55}{4} - 3B_{ij}^* - 4A_{ij}^*\right) \qquad i \neq j \tag{10b}$$

where

$$\lambda_{ij} = \frac{75R}{64N_A} \frac{\sqrt{\pi(M_i + M_j)RT/2M_iM_j}}{\pi\bar{\Omega}_{ij}^{(2,2)}} = \frac{15}{4} R \left(\frac{M_i + M_j}{2M_iM_j}\right) \eta_{ij} \tag{10c}$$

and

$$B_{ij}^* = \frac{5\bar{\Omega}_{ij}^{(1,2)} - 4\bar{\Omega}_{ij}^{(1,3)}}{\bar{\Omega}_{ij}^{(1,1)}} \tag{10d}$$

The $\bar{\Omega}_{ij}^{(1,2)}$ and $\bar{\Omega}_{ij}^{(1,3)}$ are cross sections similar to the $\bar{\Omega}_{ij}^{(1,1)}$ and $\bar{\Omega}_{ij}^{(2,2)}$ but are not associated with any particular transport property.

The preceding result for λ_{trans} represents the total thermal conductivity of a mixture of inert monatomic gases, species without internal structure. For polyatomic gases, Monchick, Yun, and Mason (ref. 17) and Monchick, Pereira, and Mason (ref. 18)

have extended the theory to include internal energy. Two assumptions were needed in order to obtain workable equations. The first assumption was that "complex collisions" (collisions involving more than a single quantum jump) could be ignored, and the second was that there was no correlation between internal energy states and relative velocities. With these assumptions plus suitable definitions of internal diffusion coefficients and relaxation times, they obtained a working equation for the thermal conductivity. They then simplified the equation to include only first-order correction terms and rearranged it to correctly give the thermal conductivity of the pure gas automatically. They expressed λ_{int} as

$$\lambda_{int} = (\lambda_{int})_{HE} + \Delta\lambda \tag{11}$$

where $(\lambda_{int})_{HE}$ is the Hirschfelder-Eucken approximation for the internal contribution to the thermal conductivity (ref. 19) and $\Delta\lambda$ is a correction term containing the inelastic effects between unlike species and some of the inelastic effects between like species. The Hirschfelder-Eucken approximation is given by

$$(\lambda_{int})_{HE} = \sum_{i=1}^{n} \left(\frac{\lambda_{int,i}}{\sum_{j=1}^{n} \frac{D_{ii}}{D_{ij}} \frac{x_j}{x_i}} \right) \tag{12}$$

where the D_{ij} are binary diffusion coefficients, the D_{ii} are self-diffusion coefficients, and $\lambda_{int,i}$ is the internal energy contribution of species i to the thermal conductivity. The $\lambda_{int,i}$ are given by (ref. 18)

$$\frac{(\lambda_{int,i})M_i}{\eta_{ii}} = \left(\frac{\rho_i D_{int,i}}{\eta_{ii}} \right) C_{int,i} - \frac{\left(\frac{2C_{int,i}}{\pi Z_i} \right) \left(\frac{5}{2} - \frac{\rho_i D_{int,i}}{\eta_{ii}} \right)^2}{1 + \left(\frac{2}{\pi Z_i} \right) \left(\frac{5}{3} \frac{C_{int,i}}{R} + \frac{\rho_i D_{int,i}}{\eta_{ii}} \right)} \tag{13}$$

where ρ_i is the density, $C_{int,i}$ the internal heat capacity, Z_i the collision number, $D_{int,i}$ a quantity which is frequently referred to as the diffusion coefficient for internal energy, and the subscript i again refers to species i. For elastic collisions, $D_{int,i}$ is reasonably well approximated by the self-diffusion coefficient (ref. 20). However, for

some molecules, this approximation is no longer valid. For example, polar molecules may exchange internal energy even at large separations. In particular, for the case of the exchange of rotational energy when the exchange is energetically resonant, Mason and Monchick have derived expressions for $D_{int,i}$ which can be expressed as (ref. 20)

$$D_{int,i} = \frac{D_{ii}}{1 + \delta_i} \tag{14}$$

They give explicit expressions for the δ_i in terms of the molecular weight, dipole moment, and moments of inertia for linear molecules and various symmetric-top molecules.

From reference 14 (p. 540),

$$\frac{\rho_i D_{ii}}{\eta_{ii}} = \frac{6}{5} A_{ii}^* \tag{15}$$

Then from equations (14) and (15),

$$\frac{\rho_i D_{int,i}}{\eta_{ii}} = \frac{6}{5}\left(\frac{A_{ii}^*}{1 + \delta_i}\right) \tag{16}$$

where $\delta_i = 0$ for nonpolar molecules.

One additional modification of equation (13) should be mentioned. Only one collision number is indicated for each species in equation (13). However, there is a different collision number for each internal energy mode. If each internal energy mode is separable and a collision number identified with each mode, then one can write (ref. 18)

$$\frac{C_{int,i}}{Z_i} = \sum_k \frac{C_{int,ki}}{Z_{ki}} \tag{17}$$

where the subscript k runs over all internal energy modes and the subscript i refers to species i. However, in practice, the rotational energy modes are usually the only ones of importance, though the vibrational ones may become important at high temperatures.

If it is assumed that the species can be characterized by one rotational collision number and by one vibrational collision number and that $D_{int,i} = D_{ii}/(1 + \delta_i)$, then from equations (13), (15), and (17) and the relationship for an ideal gas, which is

$$C_{int,i} = C_{p,i} - \frac{5}{2}R \tag{18}$$

the following is obtained:

$$\frac{(\lambda_{int,i})M_i}{\eta_{ii}} = \frac{6}{5}A_{ii}^*\left(C_{p,i} - \frac{5}{2}R\right) - \frac{\left(\frac{C_{rot,i}}{Z_{rot,i}} + \frac{C_{vib,i}}{Z_{vib,i}}\right)\left(\frac{5}{2} - \frac{6}{5}A_{ii}^*\right)^2 R}{\frac{\pi R}{2} + \left(\frac{C_{rot,i}}{Z_{rot,i}} + \frac{C_{vib,i}}{Z_{vib,i}}\right)\left[\frac{5}{3} + \frac{6/5A_{ii}^*}{(c_p/R) - (5/2)}\right]} \tag{19}$$

Equation (19) is written for nonpolar gases. For polar molecules, A_{ii}^* is replaced by $A_{ii}^*/(1 + \delta_i)$. To transform the denominator of equation (12), the following relationship is used (ref. 14, p. 530):

$$D_{ij} = \frac{3}{5}\left(\frac{M_i + M_j}{M_i M_j}\right)\left(\frac{RT}{P}\right)A_{ij}^*\eta_{ij} \tag{20}$$

When this equation is substituted into equation (12), the result is

$$(\lambda_{int})_{HE} = \sum_{i=1}^{n} \frac{\lambda_{int,i}}{\sum_{j=1}^{n} \frac{A_{ii}^*}{A_{ij}^*}\left(\frac{2M_j}{M_i + M_j}\right)\frac{\eta_{ii}}{\eta_{ij}}\frac{x_j}{x_i}} \tag{21}$$

The denominator contains quantities which have been previously defined. The computer program uses equation (21) with $\lambda_{int,i}$ obtained from equation (19). Again, for polar molecules, A_{ii}^* is replaced by $A_{ii}^*/(1 + \delta_i)$. The program does not calculate the δ_i. It is assumed that the A_{ii}^* are provided in a form which is suitable for direct use in equations (19) and (21).

Monchick, Pereira, and Mason (ref. 18) have compared calculated results for some binary mixtures with experimental measurements in order to determine the effect of including relaxation effects. Equation (11) was used along with the internal thermal conductivity of a pure species $\lambda_{int,i}$ expressed in the form

$$\lambda_{int,i} = \lambda_{exp,i} - \lambda_{monatomic,i} = \lambda_{exp,i} - \frac{15}{4}\frac{R}{M}\eta_{ii} \tag{22}$$

At the temperatures of the experimental measurements, only rotational relaxation was important. In general, satisfactory agreement was obtained between experiment and the theory of binary mixtures. Their results showed that the calculations were relatively insensitive to the inelastic collision corrections, provided that as the mole fraction of one species reached zero the calculated results were forced to agree with the experimental value of the pure gas for the other species. They concluded that for most purposes it was satisfactory to neglect inelastic effects in the mixture between different species, but that inelastic effects must be included in the calculations of the pure species. In other words, to a good approximation, $\Delta\lambda$ can be ignored in equation (11). A further consideration is that relaxation information between unlike species is almost completely lacking (ref. 18). In view of the preceding considerations the present program assumes $\Delta\lambda = 0$, and thus equation (21) is the only term contributing to equation (11).

The third and final term in equation (8) represents the contribution from chemical reaction. For a mixture of nonreacting gases (frozen mixture), this term is zero. But when chemical reactions occur, there is a contribution to the thermal conductivity. A general expression has been derived (refs. 21 and 22) for the contribution to the conductivity when local chemical equilibrium exists in a mixture of reacting gases:

$$\lambda_{reaction} = R\sum_{i=1}^{\nu}\left(\frac{\Delta H_i}{RT}\right)\lambda_{r,i} \tag{23}$$

where ν is the total number of chemical reactions and ΔH_i is the heat of reaction expressed as

$$\Delta H_i = \sum_{k=1}^{n} a_{ik}H_k \qquad i = 1,2,\ldots,\nu \tag{24}$$

In equation (24) the a_{ik} are the stoichiometric coefficients written for the chemical reactions involving species A_k as follows

$$\sum_{k=1}^{n} a_{ik}A_k = 0 \qquad i = 1,2,\ldots,\nu \tag{25}$$

The $\lambda_{r,i}$ are found by solving a set of simultaneous linear equations

$$\sum_{j=1}^{\nu} g_{ij}\lambda_{r,j} = \frac{\Delta H_i}{RT} \qquad i = 1, 2, \ldots, \nu \tag{26}$$

where the g_{ij} are given by

$$g_{ij} = \sum_{k=1}^{n-1} \sum_{l=k+1}^{n} \left(\frac{RT}{PD_{kl}} x_k x_l\right)\left(\frac{a_{ik}}{x_k} - \frac{a_{il}}{x_l}\right)\left(\frac{a_{jk}}{x_k} - \frac{a_{jl}}{x_l}\right) \tag{26a}$$

Rearranging equation (20) gives

$$\frac{RT}{PD_{kl}} = \frac{5M_k M_l}{3A^*_{kl}\eta_{kl}(M_k + M_l)}$$

which is the form of RT/PD_{kl} used in the program to evaluate g_{ij} in equation (26a). The sum of equations (9), (21), and (23) gives the total thermal conductivity of the gas mixture.

Specific Heat

The specific heat given in the transport properties table is calculated from the equation of reference 23

$$c_{p,eq} = c_{p,frozen} + c_{p,reaction} \tag{27}$$

where

$$c_{p,frozen} = \frac{\sum_{i=1}^{n} x_i C_{p,i}}{\sum_{i=1}^{n} x_i M_i} = \frac{1}{M}\sum_{i=1}^{n} x_i C_{p,i} \tag{27a}$$

and $c_{p,\text{reaction}}$ is found from an equation very similar to that for calculating $\lambda_{\text{reaction}}$ (eq. (23))

$$c_{p,\text{reaction}} = \frac{R}{M} \sum_{i=1}^{\nu} \left(\frac{\Delta H_i}{RT} \right) X_i \tag{28}$$

The X_i are found by solving the following set of linear equations:

$$\sum_{j=1}^{\nu} d_{ij} X_i = \frac{\Delta H_i}{RT} \qquad i = 1, 2, \ldots, \nu \tag{29}$$

where the d_{ij} are given by

$$d_{ij} = \sum_{k=1}^{n-1} \sum_{l=k+1}^{n} x_k x_l \left(\frac{a_{ik}}{x_k} - \frac{a_{il}}{x_l} \right) \left(\frac{a_{jk}}{x_k} - \frac{a_{jl}}{x_l} \right)$$

Equation (28) is different from, but equivalent to, that given in reference 1. It is also very similar to the equation (from refs. 21 and 22) for calculating $\lambda_{\text{reaction}}$ (eq. (23)). The only difference from equation (23) is that the (RT/PD_{kl}) term is missing in the d_{ij} coefficients. Consequently, it provides a means for checking for errors in the transport calculations, especially $\lambda_{\text{reaction}}$.

Agreement between the specific heat in the thermodynamic calculations and the specific heat in the transport calculations indicates that the transport calculations proceeded satisfactorily. However, as mentioned earlier in the section DESCRIPTION OF PROGRAM OUTPUT, differences do frequently occur for perfectly valid reasons. First, if condensed phases appear in the composition there will be some differences, because the specific heat listed in the results of the thermodynamic calculations includes condensed and gas phases, whereas the specific heat listed in the results of the transport calculations includes only the gas phase. The other reason is that sometimes not all the species appearing in the results of the thermodynamic calculations will be used in the transport calculations. This occurs because, as explained previously, only 20 gaseous species are included in the transport calculations and, among these, all the elements in the chemical system are initially included. The reason for including the elements was discussed in the section describing subroutine INPUT.

Remaining Properties

The equations for the remaining properties are summarized as follows: The frozen and equilibrium Prandtl numbers are

$$Pr_{frozen} = \frac{(c_{p,frozen})(\eta_{mixture})}{\lambda_{frozen}} \tag{30}$$

$$Pr_{eq} = \frac{(c_{p,eq})(\eta_{mixture})}{\lambda_{mixture}} \tag{31}$$

For the generalized Lewis number, as defined by Brokaw (ref. 24)

$$Le = \frac{(\lambda_{reaction})(c_{p,frozen})}{(\lambda_{frozen})(c_{p,reaction})} \tag{32}$$

A few other thermodynamic properties for the gas phase (molecular weight, enthalpy, and density) are included in the punched-card output but not in the printed output:

$$M = \sum_{i=1}^{n} x_i M_i \tag{33}$$

$$H = \sum_{i=1}^{n} x_i H_i \tag{34}$$

$$\rho = \frac{PM}{RT} \tag{35}$$

Estimation Techniques

The final subject concerns the equations used to estimate the transport cross-section data when these data are missing from the TRANSPORT data library (physical tape 4). When this occurs, empirical rules are used. For interactions involving molecules of different species, the rules suggested from the analogy to a rigid sphere (ref. 25) are

$$\bar{\Omega}_{ij}^{(2,2)} = \frac{1}{4}\left[\bar{\Omega}_{ii}^{(2,2)} + 2\sqrt{\bar{\Omega}_{ii}^{(2,2)}\bar{\Omega}_{jj}^{(2,2)}} + \bar{\Omega}_{jj}^{(2,2)}\right] \tag{36}$$

$$A_{ij}^{*} = \frac{1}{2}\left(A_{ii}^{*} + A_{jj}^{*}\right) \tag{37}$$

$$B_{ij}^{*} = \frac{1}{2}\left(B_{ii}^{*} + B_{jj}^{*}\right) \tag{38}$$

For molecules composed of hard rigid spheres the preceding equations are exact ($A_{ij}^{*} = B_{ij}^{*} = 1$).

For interactions involving molecules of the same species, an empirical relation was derived from the experimental and theoretical transport data of the pure species. This relation should not be considered as a means for providing missing data, but rather as a means for estimating cross sections of the correct order of magnitude, in order that the calculations will proceed smoothly. Problems might occur, such as division by zero, if the assigned storage locations for cross sections were allowed to remain empty. Only species for which information on transport data were available over a large temperature range were used in the analysis. These included species such as He, Ne, Ar, Kr, Xe, N, O, N_2, O_2, H_2, CO_2, and H_2O. The empirical relationship is

$$\bar{\Omega}_{ii}^{(2,2)} = \ln\left(320\,\frac{M_i^4}{T^{1.4}}\right) \tag{39}$$

where $\bar{\Omega}_{ii}^{(2,2)}$ is given in the units of square angstroms. The largest errors in equation (39) occurred for species of very low molecular weight. For very high temperatures or low molecular weights, $\bar{\Omega}_{ii}^{(2,2)}$ can become negative. In order to avoid this, $\bar{\Omega}_{ii}^{(2,2)} = 1$ was arbitrarily assigned as the smallest allowable value. For all conditions where $\bar{\Omega}_{ii}^{(2,2)}$ calculated by equation (39) is less than unity, it is set equal to unity.

The A_{ii}^{*} and B_{ii}^{*} generally show only a very slight temperature dependence and usually are close to unity. Consequently, both were set equal to 1 for all temperatures. This is also consistent with equations (37) and (38) in that this approximation is exact for molecules composed of hard rigid spheres.

Also, for each species, relaxation data are needed (Z_i), and these data are often lacking. If relaxation data for the species are not found in the tape library, the program uses the Hirschfelder-Eucken approximation (ref. 19), which is equivalent to letting $Z_{rot} = Z_{vib} = \infty$ in equation (19). There is no scheme for estimating collision numbers included in the program.

SOURCES OF TRANSPORT AND RELAXATION DATA

Sources of the transport cross-section data included with the program are given in table VIII. The data are in the nature of a preliminary set of input. In order to provide data for the large number of interactions needed in a general program, data included with the program were generally obtained directly from the literature. For the most part, the data were not examined critically, and so are not necessarily the most recent or most accurate data. There is one important exception, however. This is the input for the inert gases. A considerable amount of high-temperature experimental viscosity and thermal conductivity data have become available for the inert gases in recent years. These data, as well as the earlier data, have been used to obtain the cross-section data included with the set of input. Molecular beam scattering data were used at the higher temperatures.

One method given in table VIII which should be commented upon is method 9, which applies to the CO interactions. From consideration of the electron configurations and molecular weights of N_2 and CO, it would be anticipated that the transport cross sections for interactions involving N_2 should be about the same as those for the corresponding interactions involving CO. In order to test this supposition, the viscosity data of N_2 were compared with the viscosity data of CO (refs. 26 and 27); and the binary diffusion data for N_2-X were compared with the binary diffusion data for CO-X (ref. 28), where X is some third species. Good agreement was obtained. This suggested the possibility that if data for an interaction involving CO were unavailable, data for the corresponding interaction involving N_2 could be used. The reverse would also be true. However, since data for the N_2 interactions are considerably more extensive than those for the CO interactions, this approximation usually amounts to a method for estimating data for interactions involving CO from the corresponding interactions involving N_2.

Although the list of interactions in table VIII is not complete, it is fairly comprehensive. An effort was made to include data for all the important species and for many of the interactions between unlike species. There are two exceptions, however. First, no data have been included for ionized species; and second, data for only a few organic molecules have been included.

Relaxation data included with the program are given in table IX. Only rotational collision numbers are included. The Hirschfelder-Eucken approximation is used for vibrational relaxation ($Z_{vib} \equiv \infty$). Most of the collision numbers given for nonpolar or slightly polar molecules were obtained by fitting the experimental thermal conductivity data to equation (22), with $\lambda_{internal}$ given by equation (19), and letting $Z_{vib} = \infty$. All Z_{rot} were assumed to be independent of temperature. (The numbers given in table IX represent average values over the entire temperature range.) There were two reasons for doing this. One reason is that calculated values of Z_{rot} are usually quite sensitive to changes in the values of the viscosity and thermal conductivity used in the calculations.

Furthermore, since the uncertainty in the thermal conductivity is sometimes rather large, it often leads to very large uncertainties in the calculated collision number. The other reason is that at higher temperatures the absence of experimental thermal conductivity data means that Z_{rot} would have to be determined by some alternate technique. A reasonable procedure would be to extrapolate Z_{rot} to higher temperatures by means of some theoretical expression for the temperature dependence. However, investigators who have studied the temperature dependence from theoretical considerations have obtained significantly different results (refs. 29 to 31). Therefore, it seemed unwise to include temperature-dependent collision numbers without even being sure of the temperature dependence of Z_{rot}. Consequently, Z_{rot} was assumed to be a constant, and the numbers listed in table IX apply to all temperatures.

In some cases the experimental thermal conductivity data indicated a Z_{rot} less than unity. However, this seems inconsistent with the general physical notion of a collision number, and so for these cases Z_{rot} was set equal to 1.

For large collision numbers the calculated thermal conductivity is insensitive to variations in the collision number. A large range of Z_{rot} will adequately fit the experimental data. It becomes difficult, if not impossible, to determine a rotational collision number by just fitting thermal conductivity data. For a Z_{rot} of about 20 or more, there is very little difference between the thermal conductivity calculated by using Z_{rot} and that calculated from the Hirschfelder-Eucken approximation ($Z_{rot} = \infty$). Consequently, when the experimental thermal conductivity data indicated rather large collision numbers, the Hirschfelder-Eucken approximation was assumed.

For some species, viscosity data were available but thermal conductivity data were not. For these species the rotational collision numbers were estimated from the expression derived by Sather and Dahler (ref. 32) for a rough sphere surrounded by an attractive square-well potential. Their results for the rotational relaxation time τ may be expressed as

$$\tau^{-1} = \frac{16}{3}\left(\frac{\rho}{m_a}\right)\sigma^2\left(\frac{\pi kT}{m_a}\right)^{1/2}\left[\frac{4I/m_a\sigma^2}{\left(1 + 4I/m_a\sigma^2\right)^2}\right]g(\sigma) \tag{40}$$

Considering only the low-density limit of the radial distribution function $g(\sigma)$ (ref. 14, p. 321)

$$g(\sigma) \cong \exp\left(\frac{\epsilon}{kT}\right) \tag{41}$$

and defining a collision number Z_{rot} as (ref. 18)

$$Z_{rot} = \left(\frac{4}{\pi}\right)\left(\frac{P\tau}{\eta}\right) \tag{42}$$

we can substitute into equation (40) to obtain a value for Z_{rot}. If we further assume that the viscosity η can be calculated from the equation for viscosity of rigid-sphere molecules (ref. 14)

$$\eta = \frac{5}{16}\frac{\left(\pi m_a kT\right)^{1/2}}{\pi\sigma^2} \tag{43}$$

and use the ideal-gas law, the rotational collision number is given by

$$Z_{rot}^{-1} = \frac{5\pi}{12}\left[\frac{4I/m_a\sigma^2}{\left(1 + 4I/m_a\sigma^2\right)^2}\right]\exp\left(\frac{\epsilon}{kT}\right) \tag{44}$$

Equation (44) can be used to calculate a collision number directly or to calculate a ratio of the collision numbers of two species. The advantage of calculating a ratio is that it enables one to make use of a species for which the rotational collision number is known. This was the procedure used in obtaining the collision numbers shown in table IX. Molecules treated in this way are indicated, along with the species of "known" Z_{rot} used to make the estimate. In this report, the collision numbers obtained by fitting thermal conductivity data are considered to be the known Z_{rot}.

The equation is temperature dependent. However, since temperature dependences are not given for the species of "known" Z_{rot}, they are not given for the calculated ones either. The temperature actually used in each calculation was an average temperature. This average temperature was found by taking the average of the temperature range used in determining the Z_{rot} of the reference species ("known" Z_{rot}).

Collision numbers for the polar gases were taken from Zeleznik and Svehla (ref. 29). These are theoretical values of Z_{rot} based on a classical calculation of rotational relaxation times. The calculated values of Z_{rot} do have a temperature dependence. These are shown in table IX.

CONCLUDING REMARKS

The program described in this report is complete as it is presented herein. However, changes may occur from time to time as the authors become aware of improved techniques for doing the calculations. Though these changes may not be published, an outside organization requesting the program automatically receives the latest version.

Improved calculational results may also be obtained with the addition of new thermodynamic and transport data or with the updating of data already included in the program. This can be done by the program user if he has data to be added or changed, or he can send for the authors' updated version of the data.

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501-24.

APPENDIX A

SYMBOLS

A_e/A_t	ratio of nozzle exit area to throat area, dimensionless
A_k	chemical formula of species k, dimensionless
A_{ij}^*	$\bar{\Omega}_{ij}^{(2,2)}/\bar{\Omega}_{ij}^{(1,1)}$, dimensionless
a	sonic velocity, m/sec
a_{ik}	stoichiometric coefficient for species k in reaction i, dimensionless
B_{ij}^*	$\left[5\bar{\Omega}_{ij}^{(1,2)} - 4\bar{\Omega}_{ij}^{(1,3)}\right]/\bar{\Omega}_{ij}^{(1,1)}$, dimensionless
b_{ij}	matrix coefficient in eq. (10), (m)(sec)(K)/J
C_F	coefficient of thrust, dimensionless
C_p	heat capacity at constant pressure, J/(kg-mole)(K)
c_{ij}	matrix coefficient in eq. (7), (m)(sec)/kg
c_p	specific heat at constant pressure, J/(kg)(K)
c^*	characteristic velocity, m/sec
D_{ij}	binary diffusion coefficient, m^2/sec
d_{ij}	matrix coefficient in eq. (29), dimensionless
F/A	fuel-to-air weight (or mass) ratio or fuel-to-oxidant weight (or mass) ratio, dimensionless
% F	percent of total fuel in total reactant by weight (or mass), dimensionless
g_{ij}	matrix coefficient in eq. (26), (m)(sec)/kg-mole
$g(\sigma)$	radial distribution function evaluated at σ, dimensionless
H	enthalpy, J/kg-mole
H_0^o	standard-state enthalpy at 0 K, J/kg-mole
ΔH	heat of reaction, J/kg-mole
$\left(\Delta H_f^o\right)_T$	heat of formation at temperature T, J/kg-mole
h	enthalpy, J/kg
I	moment of inertia, (kg)(m^2)
I_{sp}	specific impulse with exit and ambient pressure equal, (N)(sec)/(kg)
I_{vac}	vacuum specific impulse, (N)(sec)/(kg)

k	Boltzmann's constant per molecule, 1.380622×10^{-23} J/K
Le	Lewis number (defined by eq. (32)), dimensionless
M	molecular weight, kg/kg-mole
m_a	molecular mass, kg
N_A	Avogadro's number, 6.022169×10^{26} molecules/kg-mole
n	number of gaseous species included in transport calculations, dimensionless
O/F	oxidant-to-fuel weight (or mass) ratio, dimensionless
P	pressure, N/m^2
P_c/P	ratio of combustion pressure to exit pressure, dimensionless
Pr	Prandtl number ($c_p\eta/\lambda$), dimensionless
R	gas constant, 8314.3 J/(kg-mole)(K) or 1.987165 cal/(g-mole)(K)
r	equivalence ratio, dimensionless
S	entropy, J/(kg-mole)(K)
S_0^o	standard-state entropy at 0 K, J/(kg-mole)(K)
s	entropy, J/(kg)(K)
T	temperature, K
U	internal energy, J/kg-mole
u_1	velocity of unshocked gas relative to incident shock front, m/sec
u_2	velocity of incident-shocked gas relative to incident shock front, m/sec
V	volume, m^3
v_2	actual velocity of incident-shocked gases in fixed coordinates, m/sec
X_i	unknown in eq. (28), dimensionless
x_i	mole fraction of species i, dimensionless
Z_i	collision number of species i, dimensionless
γ	isentropic exponent $(\partial \ln P/\partial \ln \rho)_S$, dimensionless
δ	correction term in eq. (14) for resonant exchange of rotational energy, dimensionless
ϵ	depth of potential energy well, J
η	viscosity, kg/(m)(sec)
η_i	unknown in eq. (6), kg/(m)(sec)

η_{ii}	viscosity of species i, kg/(m)(sec)
η_{ij}	defined quantity (see eq. (7c)), kg/(m)(sec)
λ	thermal conductivity, J/(m)(sec)(K)
λ_j	unknown in eq. (9), J/(m)(sec)(K)
λ_{ij}	defined quantity (see eq. (10c)), J/(m)(sec)(K)
$\lambda_{r,i}$	unknown in eq. (23), kg-mole/(m)(sec)
$\Delta\lambda$	correction term involving relaxation effects, J/(m)(sec)(K)
ν	number of chemical reactions, dimensionless
$\pi\bar{\Omega}(l,s)$	collision cross section (equivalent to $\pi\sigma^2\Omega^{(2,2)*}$ of ref. 14), m^2
ρ	density, kg/m^3
σ	molecular diameter in eq. (40), m
τ	rotational relaxation time, sec

Subscripts:

eq	equilibrium
exp	experimentally measured value
frozen	chemically frozen (nonreacting)
HE	Hirschfelder-Eucken
i,j,k,l	index for species or reaction number
int	pertaining to internal energy modes
mixture	for the mixture
monatomic	translational energy contribution for a single species
P	at constant pressure
reaction	chemical reaction contribution
rot	rotational
S	at constant entropy
T	at constant temperature
trans	translational
vib	vibrational

Superscript:

o	standard state

APPENDIX B

VARIABLES, INDICES, AND CONSTANTS USED IN TRANSPORT SUBROUTINES

FORTRAN symbol	Dimension	Common label[a]	Transport subroutines used[b]	Description and comments[c]
A	10,100	SPECES	INPUT	Stoichiometric coefficient A(i,j) of element i in species j
ANS	15	TRANS	TRANSP OUT	Output results (each ANS equivalenced to a particular property)
ANSR	3	INTERP	INPUT LGRNGE	Answer vector from Lagrange interpolation
ASTAR	20,20	TRANS	TRANSP INPUT	$\bar{\Omega}^{(2,2)}_{ij}/\bar{\Omega}^{(1,1)}_{ij}$, A^*_{ij}
ATOM	3,101	MISC	INPUT	For atom j ATOM(1,j) = atomic symbol ATOM(2,j) = atomic weight ATOM(3,j) = atomic valence
AVGDRO	1	DATA STATEMENT	TRANSP	Avogadro's Number (without the exponent 10^{26})
BIGEN	1	----------	INPUT	Test number in finding largest EN
BOLTZ	1	DATA STATEMENT	TRANSP	Boltzmann's Constant (without the exponent 10^{-23})
BSTAR	20,20	TRANS	TRANSP INPUT	$(5\bar{\Omega}^{(1,2)}_{ij} - 4\bar{\Omega}^{(1,3)}_{ij})/\bar{\Omega}^{(1,1)}_{ij}$, B^*_{ij}
CHECK	20	DIMENSION STATEMENT	TRANSP	Check of results from GAUSS solution, double precision
COEFF	1	----------	INPUT	Stoichiometric coefficient of species to be eliminated (in the reaction to be eliminated)
CONST	1	----------	TRANSP	Coefficient in η_{ij}, $5/16(10^{54}k/\pi N_A)^{1/2}$
CPEQ	1	EQUIVALENCE STATEMENT	TRANSP	Equilibrium specific heat of mixture, $c_{p,eq}$
CPFROZ	1	EQUIVALENCE STATEMENT	TRANSP	Frozen specific heat of mixture, $c_{p,frozen}$
CPREAC	1	EQUIVALENCE STATEMENT	TRANSP	Reaction specific heat of mixture, $c_{p,reaction}$
CPRR	20	TRANS	TRANSP	Dimensionless heat capacity, C_p/R
CVIBR	20	TRANS	TRANSP INPUT	Vibrational heat capacity, C_{vib}
DELH	17	DIMENSION STATEMENT	TRANSP	Heat of reaction, $\Delta H/RT$
DENSTY	1	EQUIVALENCE STATEMENT	TRANSP	Gas density of mixture used in transport calculations, ρ
EN	100,13	SPECES	INPUT	EN(i,j) - kg-moles of species i per kg of mixture for point j
ENTLPY	1	EQUIVALENCE STATEMENT	TRANSP OUT	Enthalpy, H
ENTRPY	1	----------	OUT	Entropy, S
ETA	20,20	DIMENSION STATEMENT	TRANSP	Quantity defined in equation (7), η_{ij}

[a] Common block is specified. If it is not in a common block, the type of statement is indicated. If it is in neither, a dash is shown.

[b] In most cases only the transport subroutines are listed. However, in some cases, it was useful to list the other routines in order to describe the application.

[c] FORTRAN IV convention is followed unless otherwise indicated. If the variable is real, integer, logical, or double precision, it is so indicated.

NOT REPRODUCIBLE

FORTRAN symbol	Dimension	Common label	Transport subroutines used	Description and comments
EQCON	1	EQUIVALENCE STATEMENT	TRANSP	Equilibrium thermal conductivity of mixture, $\lambda_{mixture}$
EQRAT	1	MISC	OUT	Equivalence ratio
FIRSTP	1	SAVED	OUT	First pressure, P
FIRSTV	1	SAVED	OUT	First volume, V
FPC	1	----------	OUT	Fuel percent, 1/(1 + OF)
FROZN	1	CONTRL	TRANSP INPUT OUT	Point is frozen if FROZN = T, logical variable
FRZCON	1	EQUIVALENCE STATEMENT	TRANSP	Frozen thermal conductivity of mixture, λ_{frozen}
G	20,21	DOUBLE	TRANSP GAUSS	Matrix coefficients, double precision
GMAT	20,21	DIMENSION STATEMENT	TRANSP	Set equal to G, used for checking results from GAUSS, double precision
HRRT	20	TRANS	TRANSP	Dimensionless enthalpy, H/RT
IATOM	3,101	DIMENSION STATEMENT EQUIVALENCE STATEMENT	INPUT	Equivalenced to ATOM, used to identify elements in calculating molecular weights
IMAT	1	INDX	TRANSP	Number of equations in GAUSS solution
IND	20	SAVED	TRANSP INPUT	Index to identify species used in transport calculations
INTCON	1	EQUIVALENCE STATEMENT	TRANSP	Internal thermal conductivity of mixture, $\lambda_{internal}$, real variable
INTRNL	1	----------	OUT	Internal energy of first point, U, real variable
ISV	1	INDX	TRANSP OUT	Used as test in controlling transport output ISV ≠ 0: more thermodynamic calculations to follow ISV = 0: end of thermodynamic calculations of problem
ITT	1	----------	OUT	Current temperature expressed as integer
IUSE	100	SPECES	SEARCH INPUT	Used as test to see if species is condensed
LEWIS	1	EQUIVALENCE STATEMENT	TRANSP OUT	Lewis number, Le, real variable
LLL	1	SAVED	OUT	Index to control spacing interval in transport output
LLMT	10	MISC	INPUT	Alphameric symbols for elements
LM	1	SAVED	OUT	Index of current point being processed in transport output
MAXNM	1	DATA STATEMENT	INPUT	Maximum number of species allowed
MAXNP	1	SAVED	TRANSP INPUT OUT	Index used in controlling transport output
MONCON	1	EQUIVALENCE STATEMENT	TRANSP	Translational thermal conductivity of mixture, λ_{trans}, real variable

FORTRAN symbol	Dimension	Common label	Transport subroutines used	Description and comments
N	1	TRANS	TRANSP INPUT OUT	Index of current point
ND	1	DATA STATEMENT	SEARCH TRANSP INPUT	Indicates end of transport data
NFZ	1	PERF	INPUT OUT	Index of freezing point
NLM	1	INDX	INPUT	Number of elements in the system
NM	1	SAVED	TRANSP INPUT	Number of species in transport calculations, n
NODATA	1	CONTRL	INPUT	If NODATA = T, message is printed out whenever cross section data are not found in the library - applies only to data for a pure species, logical variable
NPT	1	INDX	TRANSP	Number of points in current set
NR	1	TRANS	TRANSP INPUT	Number of chemical reactions, ν
NS	1	INDX	SEARCH TRANSP INPUT	Number of species in the thermodynamic calculations
NSP	1	----------	INPUT	Special index used to change A array to add an element which has been omitted through use of an OMIT card
NTAB	100	TRANS	TRANSP INPUT	Code to specify type of data used in transport calculations: = 0 if relaxation data = 1 if transport cross sections
NTB	1	----------	SEARCH TRANSP INPUT	
NTP	1	----------	SEARCH TRANSP INPUT LGRNGE	Number of entries in table of transport or relaxation data (data stored in TABLES)
NTT	100	TRANS	TRANSP INPUT	
OF	1	MISC	OUT	Oxidant-to-fuel weight ratio
OMEGA	20,20	TRANS	TRANSP INPUT	Viscosity cross section, $\bar{\Omega}^{(2,2)}$
PI	1	DATA STATEMENT	TRANSP	π, 3.14159265
PP	1	MISC	TRANSP OUT	Pressure of current point
PPP	13	POINTS	TRANSP OUT	Pressure schedule for output
PREQ	1	EQUIVALENCE STATEMENT	TRANSP	Equilibrium Prandtl number of mixture, Pr_{eq}
PRFROZ	1	EQUIVALENCE STATEMENT	TRANSP	Frozen Prandtl number of mixture, Pr_{frozen}
PUNCH	1	CONTRL	OUT	If PUNCH = T output is included on punched cards, logical variable
R	1	MISC	TRANSP OUT	Universal gas constant, 1.987165 cal/(g-mole)(K) or 8.31430 J/(kg-mole)(K)

FORTRAN symbol	Dimension	Common label	Transport subroutines used	Description and comments
REACON	1	EQUIVALENCE STATEMENT	TRANSP	Reaction thermal conductivity of mixture, $\lambda_{reaction}$
RELXTN	20	TRANS	TRANSP	Temporary storage used in calculating $\lambda_{internal}$
ROTM	20	TRANS	TRANSP INPUT	Number of rotational degrees of freedom
ROTN	1	----------	SEARCH TRANSP	
ROTNM	80	TRANS	TRANSP INPUT	
RPVT	1	DATA STATEMENT	TRANSP	Universal gas constant, 82.0562 $(cm^3)(atm)/(g\text{-}mole)/(K)$
SPECE	2,3	DIMENSION STATEMENT	SEARCH	Alphameric identification of current interaction, integer variable
		TRANS	TRANSP	
SPECIE	100,2,3	TRANS	TRANSP INPUT	Alphameric identification of interaction which is put in core storage with TABLES, integer variable
STC	17,20	TRANS	TRANSP INPUT	Table of stoichiometric coefficients, a_{ik}
STCF	17,20	TRANS	INPUT	Intermediate storage of stoichiometric coefficients
STCOEF	20	TRANS	INPUT	Result of dividing stoichiometric coefficients of each species (in the reaction to be eliminated) by COEFF
STORE	52,16	SAVED	OUT	Temporary storage of transport calculations, while thermodynamic calculations are continued
SUB	100,3	SPECES	SEARCH TRANSP INPUT	Alphameric name of species included in thermodynamic calculations, integer variable
TABLES	100,20,3	TRANS	TRANSP INPUT	Tables of cross sections and relaxation data
TABLS	20,3	DIMENSION STATEMENT	SEARCH	
TEM	100,20	TRANS	TRANSP INPUT	Temperature schedule for TABLES
TEMPR	20	DIMENSION STATEMENT	SEARCH	Temperature schedule for TABLS
TESTEN	1	----------	INPUT	Smallest EN allowed in transport calculations
TRNSPT	1	CONTRL	LINK	If TRNSPT = F transport calculations are omitted, logical variable
TT	1	MISC	TRANSP INPUT OUT LGRNGE	Temperature of current point
TTT	13	POINTS	TRANSP	Temperature schedule for output
VISC	1	EQUIVALENCE STATEMENT	TRANSP	Viscosity of mixture, $\eta_{mixture}$
WM	13	POINTS	INPUT	Molecular weight of the mixture in thermodynamic calculations
WMOL	20	SAVED	TRANSP INPUT	Molecular weight of pure species, M_i
WTMOL	1	EQUIVALENCE STATEMENT	TRANSP	Molecular weight of the mixture in transport calculations, M

FORTRAN symbol	Dimension	Common label	Transport subroutines used	Description and comments
X	20	DOUBLE	TRANSP GAUSS	Answer region for matrix solution, double precision
XS	20	SAVED	TRANSP INPUT	Mole fraction of species used in transport calculations
XSKL	20,20	DIMENSION STATEMENT	TRANSP	$(XS(k) \cdot XS(l))^{-1}$
Y	20,3	INTERP	INPUT LGRNGE	Table in subroutine LGRNGE interpolation
Z	20	INTERP	INPUT LGRNGE	Argument in subroutine LGRNGE interpolation
ZROT	20	TRANS	TRANSP INPUT	Rotational collision number, Z_{rot}
ZVIB	20	TRANS	TRANSP INPUT	Vibrational collision number, Z_{vib}

APPENDIX C

PROGRAM LISTING

```
C
C     MAIN PROGRAM                                                          LINK    1
C                                                                           LINK    2
C     LINKS SUBROUTINES FOR THERMODYNAMIC AND TRANSPORT CALCULATIONS FORLINK    3
C                                                                           LINK    4
      DOUBLE PRECISION G,X                                                  LINK    5
C                                                                           LINK    6
      REAL MIX(15)                                                          LINK    7
      INTEGER SPECE                                                         LINK    8
      INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END,SUB                LINK    9
C                                                                           LINK   10
      LOGICAL SHOCK,MMHG,UV,IC,DETN,SIUNIT,EUNITS,NSQM                      LINK   11
      LOGICAL HP,SP,TP,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV          LINK   12
      LOGICAL FA,OF,ERATIO,FPCT,OTTO                                        LINK   13
      LOGICAL TRNSPT,FROZN,PUNCH,NODATA                                     LINK   14
C                                                                           LINK   15
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),         LINK   16
     1 GAMMAS(13),P(26),T(52),V(26),PPP(13),WM(13),SONVEL(13),TTT(13),      LINK   17
     2 VLM(13),TOTN(13)                                                     LINK   18
      COMMON /SPECES/COEF(2,7,100),S(100),H0(100),DELN(100),DUMMY(100),     LINK   19
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)       LINK   20
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),LINK   21
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),          LINK   22
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),             LINK   23
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),LINK   24
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)          LINK   25
      COMMON /DOUBLE/ G(20,21), X(20)                                       LINK   26
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,       LINK   27
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,    LINK   28
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,    LINK   29
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT               LINK   30
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),            LINK   31
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,          LINK   32
     2 APPL,ARATIO,ELN                                                      LINK   33
      COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,        LINK   34
     1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,                LINK   35
     2 FIRSTP,FIRSTV                                                        LINK   36
      COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA                              LINK   37
C                                                                           LINK   38
C                                                                           LINK   39
      LM = 0                                                                LINK   40
      MAXNP = 0                                                             LINK   41
      NEWR = .FALSE.                                                        LINK   42
      NLS = 0                                                               LINK   43
    1 CALL MAIN                                                             LINK   44
    2 IF(NPT.EQ.0) GO TO 1                                                  LINK   45
      IF(.NOT.RKT.AND..NOT.SHOCK) GO TO 7                                   LINK   46
      IF(.NOT.EQL) FROZN = .TRUE.                                           LINK   47
      IF(EQL) FROZN = .FALSE.                                               LINK   48
    7 IF(.NOT.TRNSPT) GO TO 8                                               LINK   49
      CALL TRANSP                                                           LINK   50
    8 IF(.NOT.RKT) GO TO 3                                                  LINK   51
      CALL ROCKT1 ($1)                                                      LINK   52
      GO TO 2                                                               LINK   53
    3 IF(.NOT.DETN) GO TO 4                                                 LINK   54
      CALL DETON1 ($1)                                                      LINK   55
      GO TO 2                                                               LINK   56
```

```
    4 IF(.NOT.SHOCK) GO TO 5                                          LINK  57
      CALL SHOK1 ($1)                                                 LINK  58
      GO TO 2                                                         LINK  59
    5 CONTINUE                                                        LINK  60
      CALL THERM1 ($1)                                                LINK  61
      GO TO 2                                                         LINK  62
      END                                                             LINK  63
```

```
C
      SUBROUTINE GAUSS                                                GAUS   1
C                                                                     GAUS   2
C     SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS                      GAUS   3
C     NUMBER OF EQUATIONS = IMAT                                      GAUS   4
C                                                                     GAUS   5
      DOUBLE PRECISION G,X,COEFX(20),SUM,Z                            GAUS   6
C                                                                     GAUS   7
      COMMON/DOUBLE/G(20,21),X(20)                                    GAUS   8
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM, GAUS   9
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, GAUS  10
     2 ICNS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, GAUS  11
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT          GAUS  12
C                                                                     GAUS  13
      DATA BIGNO/1.E+38/                                              GAUS  14
C                                                                     GAUS  15
C     BEGIN ELIMINATION OF NNTH VARIABLE                              GAUS  16
C                                                                     GAUS  17
      IUSE1 = IMAT+1                                                  GAUS  18
    6 DO 45  NN=1,IMAT                                                GAUS  19
      IF(NN-IMAT)  8,83,8                                             GAUS  20
   83 IF(G(NN,NN)) 31,23,31                                           GAUS  21
C                                                                     GAUS  22
C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                      GAUS  23
C                                                                     GAUS  24
    8 DO 18  I=NN,IMAT                                                GAUS  25
      COEFX(I) = BIGNO                                                GAUS  26
      IF(G(I,NN).EQ.0.)  GO TO 18                                     GAUS  27
      COEFX(I) = 0.                                                   GAUS  28
      DO 10 J=NN,IUSE1                                                GAUS  29
      SUM = G(I,J)                                                    GAUS  30
      IF(SUM.LT.0.)  SUM=-SUM                                         GAUS  31
      IF(J.NE.NN)  GO TO 9                                            GAUS  32
      Z = SUM                                                         GAUS  33
      GO TO 10                                                        GAUS  34
    9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                               GAUS  35
   10 CONTINUE                                                        GAUS  36
      COEFX(I) = COEFX(I)/Z                                           GAUS  37
   18 CONTINUE                                                        GAUS  38
C                                                                     GAUS  39
C     LOCATE ROW WITH SMALLEST MAXIMUM COEFFICIENT                    GAUS  40
C                                                                     GAUS  41
      TEMP = BIGNO                                                    GAUS  42
      I=0                                                             GAUS  43
   20 DO 22  J=NN,IMAT                                                GAUS  44
      IF (COEFX(J)-TEMP) 87,22,22                                     GAUS  45
   87 TEMP=COEFX(J)                                                   GAUS  46
      I=J                                                             GAUS  47
   22 CONTINUE                                                        GAUS  48
      IF(I) 28,23,28                                                  GAUS  49
```

```
C                                                                       GAUS  50
C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH       GAUS  51
C     VARIABLE FROM THE REMAINING EQUATIONS                             GAUS  52
C                                                                       GAUS  53
C     INTERCHANGE EQUATIONS I AND NN                                    GAUS  54
C                                                                       GAUS  55
   28 IF(NN-I) 29,31,29                                                 GAUS  56
   29 DO 30 J=NN,IUSE1                                                  GAUS  57
      Z=G(I,J)                                                          GAUS  58
      G(I,J)=G(NN,J)                                                    GAUS  59
      G(NN,J)=Z                                                         GAUS  60
   30 CONTINUE                                                          GAUS  61
C                                                                       GAUS  62
C     DIVICE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH      GAUS  63
C     VARIABLE FROM THE REMAINING EQUATIONS                             GAUS  64
C                                                                       GAUS  65
   31 K = NN + 1                                                        GAUS  66
      DO 36 J = K, IUSE1                                                GAUS  67
      IF(G(NN,NN).EQ.0.)  GO TO 23                                      GAUS  68
      G(NN,J) = G(NN,J) / G(NN,NN)                                      GAUS  69
   36 CONTINUE                                                          GAUS  70
      IF(K-IUSE1) 88,45,88                                              GAUS  71
   88 DO 44  I=K,IMAT                                                   GAUS  72
   40 DO 44 J = K,IUSE1                                                 GAUS  73
      G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                                 GAUS  74
   44 CONTINUE                                                          GAUS  75
   45 CONTINUE                                                          GAUS  76
C                                                                       GAUS  77
C     BACKSOLVE FOR THE VARIABLES                                       GAUS  78
C                                                                       GAUS  79
      K = IMAT                                                          GAUS  80
   47 J = K + 1                                                         GAUS  81
      X(K) = 0.0D0                                                      GAUS  82
      SUM = 0.0                                                         GAUS  83
      IF(IMAT-J)  51,48,48                                              GAUS  84
   48 DO 50  I=J,IMAT                                                   GAUS  85
      SUM = SUM + G(K,I)* X(I)                                          GAUS  86
   50 CONTINUE                                                          GAUS  87
   51 X(K) = G(K,IUSE1) - SUM                                           GAUS  88
      K = K - 1                                                         GAUS  89
      IF(K) 47,151,47                                                   GAUS  90
   23 IMAT = IMAT-1                                                     GAUS  91
  151 RETURN                                                            GAUS  92
      END                                                               GAUS  93
```

```
C                                                                       MAIN   1
      SUBROUTINE MAIN                                                   MAIN   2
C                                                                       MAIN   3
C     MAIN PROGRAM FOR THERMODYNAMIC CALCULATIONS                       MAIN   4
C                                                                       MAIN   5
      DOUBLE PRECISION G,X                                              MAIN   6
C                                                                       MAIN   7
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      MAIN   8
C     IBM 360 MACHINES ONLY                                             MAIN   9
C                                                                       MAIN  10
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                 MAIN  11
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN
```

```
C                                                                       MAIN  12
      REAL MIX(15)                                                      MAIN  13
      INTEGER SPECE                                                     MAIN  14
      INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END,SUB            MAIN  15
      LOGICAL SHOCK,MMHG,UV,IC,DETN,SIUNIT,EUNITS,NSQM,CALCH            MAIN  16
      LOGICAL HP,SP,TP,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV      MAIN  17
      LOGICAL FA,OF,ERATIO,FPCT,OTTO                                    MAIN  18
      LOGICAL TRNSPT,FROZN,PUNCH,NODATA                                 MAIN  19
C                                                                       MAIN  20
      DIMENSION OMIT(3,3),NCD(4),ENSERT(3,3),RHO(26),LVP(2),VM(2),      MAIN  21
     1 VL(26),DAT(22)                                                   MAIN  22
      DIMENSION SPECE(2,3),TEMPR(20),TABLS(20,3)                        MAIN  23
C                                                                       MAIN  24
      COMMON   SPECE , TEMPR , TABLS                                    MAIN  25
C                                                                       MAIN  26
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     MAIN  27
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  MAIN  28
     2 VLM(13),TOTN(13)                                                 MAIN  29
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), MAIN  30
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   MAIN  31
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),MAIN  32
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      MAIN  33
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         MAIN  34
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FCX(15),DENS(15),MAIN  35
     4 RHOP,RMM(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      MAIN  36
      COMMON /DOUBLE/ G(20,21), X(20)                                   MAIN  37
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   MAIN  38
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, MAIN  39
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, MAIN  40
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            MAIN  41
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        MAIN  42
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       MAIN  43
     2 APPL,ARATIO,ELN                                                  MAIN  44
      COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA                          MAIN  45
C                                                                       MAIN  46
      EQUIVALENCE (OMIT,ENLN),(ENSERT,DELN),(OXF,MIX),                  MAIN  47
     1 (OF,CXFL),(RHO,P,VL),(SO,SO),(OTTO,CPCVFR),(DATA,DAT)            MAIN  48
C                                                                       MAIN  49
      DATA MIT/4HOMIT/,BLANK/1H /, PSIA/4HPSIA/,REAC/4HREAC/,IZ/2H00/,  MAIN  50
     1 NMLT/4HNAME/,IE/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/,     MAIN  51
     2 GAS/1HG/,ND/4HLAST/                                              MAIN  52
C                                                                       MAIN  53
      NAMELIST/INPT2/KASE,T,P,PSIA,MMHG,NSQM,V,RHO,ERATIO,OF,FPCT,FA,   MAIN  54
     1MIX,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,CR,SO,SO,IONS,IDEBUG,   MAIN  55
     2TRACE,SIUNIT,EUNITS,TRNSPT,FROZN,PUNCH,NODATA                     MAIN  56
C                                                                       MAIN  57
      NEWR = .FALSE.                                                    MAIN  58
C                                                                       MAIN  59
    1 WRITE(6,400)                                                      MAIN  60
  400 FORMAT(1H1)                                                       MAIN  61
      RR = 8314.3                                                       MAIN  62
      R = RR/4184.                                                      MAIN  63
  203 READ (5,204) (DATA(I),I=1,15)                                     MAIN  64
  204 FORMAT(5(3A4,3X))                                                 MAIN  65
      WRITE (6,2045)(DATA(I),I=1,15)                                    MAIN  66
 2045 FORMAT(1X,5(3A4,3X))                                              MAIN  67
      IF(DATA(1).EQ.THRM)  GO TO 90                                     MAIN  68
      IF(DATA(1).EQ.REAC)  GO TO 11                                     MAIN  69
      IF (DATA(1).EQ.MIT) GO TO 205                                     MAIN  70
      IF (DATA(1).EQ.INSERT) GO TO 180                                  MAIN  71
      IF(DATA(1).EQ.NMLT)  GO TO 210                                    MAIN  72
      IF(DATA(1).EQ.BLANK) GO TO 203                                    MAIN  73
 1023 WRITE(6,1024)                                                     MAIN  74
 1024 FORMAT(40HOERROR IN ABOVE CARD.  CONTENTS IGNORED. )              MAIN  75
      GO TO 203                                                         MAIN  76
```

```
   11 NSERT = 0                                                          MAIN  77
      MOLES = .FALSE.                                                    MAIN  78
      CALL REACT                                                         MAIN  79
      IF(NLM.EQ.0)  WRITE(6,52)                                          MAIN  80
   52 FORMAT(24HCERROR IN REACTANT CARDS)                                MAIN  81
      CALCH = .FALSE.                                                    MAIN  82
      DO 755 N=1,NREAC                                                   MAIN  83
      IF(NAME(N,5).EQ.IZ)  CALCH=.TRUE.                                  MAIN  84
  755 CONTINUE                                                           MAIN  85
      GO TO 202                                                          MAIN  86
C                                                                        MAIN  87
C     READ THERMO AND TRANSPORT DATA FROM CARDS AND STORE ON TAPE 4      MAIN  88
C                                                                        MAIN  89
   90 NEWR = .TRUE.                                                      MAIN  90
      REWIND 4                                                           MAIN  91
      READ(5,5) TLOW,TMID,THIGH                                          MAIN  92
    5 FORMAT (3F10.3)                                                    MAIN  93
      WRITE (4,5) TLOW,TMID,THIGH                                        MAIN  94
   97 READ (5,10)(DAT(I),I=1,16),NCD(1)                                  MAIN  95
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)                        MAIN  96
      IF(DATA(1).EQ.BLANK) DATA(1)=END                                   MAIN  97
      WRITE (4,10)(DAT(I),I=1,16)                                        MAIN  98
      IF(DATA(1).NE.END)  GO TO 18                                       MAIN  99
      GO TO 13                                                           MAIN 100
   18 READ(5,20)(DAT(I),I=1,5),NCD(2),(DAT(J),J=6,10),NCD(3),(DAT(K),    MAIN 101
     1K=11,14),NCD(4)                                                    MAIN 102
   20 FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)                             MAIN 103
      WRITE (4,21)(DAT(I),I=1,14)                                        MAIN 104
   21 FORMAT(5E15.8/5E15.8/4E15.8)                                       MAIN 105
      DO 25  I=1,4                                                       MAIN 106
      IF(NCD(I).EQ.I)  GO TO 25                                          MAIN 107
      WRITE(6,22) (DATA(J),J=1,3)                                        MAIN 108
   22 FORMAT(28HCERROR IN ORDER OF CARDS FOR ,3A4)                       MAIN 109
   25 CONTINUE                                                           MAIN 110
      GO TO 97                                                           MAIN 111
C                                                                        MAIN 112
C     TRANSPORT DATA CARDS                                               MAIN 113
C                                                                        MAIN 114
   13 READ(5,14) ((SPECE(I,L),L=1,3),I=1,2),NTP,NTB,ROTN                 MAIN 115
   14 FORMAT(2(3A4,6X),2I5,F24.1)                                        MAIN 116
      WRITE(4) ((SPECE(I,L),L=1,3),I=1,2),NTP,NTB,ROTN                   MAIN 117
      IF(SPECE(1,1).EQ.ND) GO TO 203                                     MAIN 118
      READ(5,15)(TEMPR(I),(TABLS(I,L),L=1,3),I=1,NTP)                    MAIN 119
      WRITE(4) (TEMPR(I),(TABLS(I,L), L=1,3),I=1,NTP)                    MAIN 120
   15 FORMAT(4F10.4)                                                     MAIN 121
      GO TO 13                                                           MAIN 122
C                                                                        MAIN 123
C                                                                        MAIN 124
C    CHECK INSERT CARDS                                                  MAIN 125
C                                                                        MAIN 126
  180 DO 185 I=4,15,3                                                    MAIN 127
      IF (DATA(I).EQ.BLANK) GO TO 185                                    MAIN 128
      NSERT = NSERT+1                                                    MAIN 129
      ENSERT(1,NSERT) = DATA(I)                                          MAIN 130
      ENSERT(2,NSERT) = DATA(I+1)                                        MAIN 131
      ENSERT(3,NSERT) = DATA(I+2)                                        MAIN 132
  185 CONTINUE                                                           MAIN 133
      GO TO 202                                                          MAIN 134
C                                                                        MAIN 135
C     CHECK OMIT CARDS                                                   MAIN 136
C                                                                        MAIN 137
  205 DO 208  I=4,15,3                                                   MAIN 138
      IF(DATA(I).EQ.BLANK) GO TO 208                                     MAIN 139
      NOMIT = NOMIT+1                                                    MAIN 140
      OMIT(1,NOMIT) = DATA(I)                                            MAIN 141
```

```
      OMIT(2,NCMIT) = DATA(I+1)                                          MAIN 142
      OMIT(3,NCMIT) = DATA(I+2)                                          MAIN 143
  208 CONTINUE                                                           MAIN 144
      NEWR= .TRUE.                                                       MAIN 145
      REWIND 4                                                           MAIN 146
      GO TO 203                                                          MAIN 147
C                                                                        MAIN 148
C     BEGIN NAMELIST INPT2                                               MAIN 149
C                                                                        MAIN 150
  210 DO 299 I=1,26                                                      MAIN 151
      P(I)= 0.                                                           MAIN 152
      V(I) = 0.                                                          MAIN 153
  299 CONTINUE                                                           MAIN 154
      DO 306 I=1,52                                                      MAIN 155
      T(I)=0.                                                            MAIN 156
  306 CONTINUE                                                           MAIN 157
      TRACE = 0.                                                         MAIN 158
      S0 = 0.                                                            MAIN 159
      V1 = 0.                                                            MAIN 160
      V2 = 0.                                                            MAIN 161
      CR = 0.                                                            MAIN 162
      RHCP = 0.                                                          MAIN 163
      KASE= 0                                                            MAIN 164
      TP = .FALSE.                                                       MAIN 165
      HP=.FALSE.                                                         MAIN 166
      SP=.FALSE.                                                         MAIN 167
      TV = .FALSE.                                                       MAIN 168
      UV = .FALSE.                                                       MAIN 169
      SV = .FALSE.                                                       MAIN 170
      OTTO = .FALSE.                                                     MAIN 171
      RKT = .FALSE.                                                      MAIN 172
      SHOCK = .FALSE.                                                    MAIN 173
      DETN = .FALSE.                                                     MAIN 174
      VOL = .FALSE.                                                      MAIN 175
      MMHG   = .FALSE.                                                   MAIN 176
      PSIA = .FALSE.                                                     MAIN 177
      NSQM = .FALSE.                                                     MAIN 178
      SIUNIT = .FALSE.                                                   MAIN 179
      EUNITS = .FALSE.                                                   MAIN 180
      IONS = .FALSE.                                                     MAIN 181
      IDEBUG = 0                                                         MAIN 182
      FA= .FALSE.                                                        MAIN 183
      OF= .FALSE.                                                        MAIN 184
      ERATIO = .FALSE.                                                   MAIN 185
      FPCT= .FALSE.                                                      MAIN 186
      TRNSPT = .TRUE.                                                    MAIN 187
      FROZN = .FALSE.                                                    MAIN 188
      PUNCH = .FALSE.                                                    MAIN 189
      NCDATA= .FALSE.                                                    MAIN 190
      DO 303 I=1,15                                                      MAIN 191
      MIX(I) = 0.                                                        MAIN 192
  303 CONTINUE                                                           MAIN 193
      NT = 1                                                             MAIN 194
      EQL = .TRUE.                                                       MAIN 195
      READ(5,INPT2)                                                      MAIN 196
      WRITE(6,INPT2)                                                     MAIN 197
      IF(.NOT.DETN.AND..NOT.SHOCK)  GO TO 1303                           MAIN 198
      DO 1300  N=1,NREAC                                                 MAIN 199
      IF(FAZ(N).NE.GAS)  GO TO 1301                                      MAIN 200
 1300 CONTINUE                                                           MAIN 201
      GO TO 1303                                                         MAIN 202
 1301 WRITE(6,1302)                                                      MAIN 203
 1302 FORMAT(60HOCONDENSED REACTANTS NOT PERMITTED IN DETN OR SHOCK PROBMAIN 204
     1LEMS)                                                              MAIN 205
      GO TO 1                                                            MAIN 206
```

```
 1302 IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV)  GO TO 304                    MAIN 207
      VOL = .TRUE.                                                      MAIN 208
      DO 1304  I=1,26                                                   MAIN 209
      IF(RHO(I).NE.0.)  VL(I) = 1./RHO(I)                               MAIN 210
      IF(V(I).NE.0.)  VL(I)=V(I)                                        MAIN 211
      IF(VL(I).EQ.0.)  GO TO 1305                                       MAIN 212
      NP = I                                                            MAIN 213
 1304 CONTINUE                                                          MAIN 214
 1305 TP = TV                                                           MAIN 215
      HP = UV                                                           MAIN 216
      SP = SV                                                           MAIN 217
      GO TO 322                                                         MAIN 218
  304 DO 305  I=1,26                                                    MAIN 219
      IF(P(I ).EQ.0.) GO TO 322                                         MAIN 220
      NP = I                                                            MAIN 221
      IF (MMHG) P(NP) = P(NP)/760.                                      MAIN 222
      IF(PSIA)  P(NP)=P(NP)/14.696C06                                   MAIN 223
      IF(NSQM) P(NP)=P(NP)/101325.                                      MAIN 224
  305 CONTINUE                                                          MAIN 225
  322 DO 307 IT = 1,52                                                  MAIN 226
      IF (T(IT).EQ.0.) GO TO 722                                        MAIN 227
      NT = IT                                                           MAIN 228
  307 CONTINUE                                                          MAIN 229
  722 DO 625 IST=1,15                                                   MAIN 230
      IF( MIX(IST).NE.0.) GO TO 323                                     MAIN 231
      IF(IST.NE.1) GO TO 745                                            MAIN 232
      WRITE(6,724)                                                      MAIN 233
  724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT  )     MAIN 234
      IF (WP(2).NE.0.) OXFL = WP(1)/WP(2)                               MAIN 235
      GO TO 333                                                         MAIN 236
  323 OXFL = MIX(IST)                                                   MAIN 237
      IF(FA) OXFL =1./MIX(IST)                                          MAIN 238
      IF(FPCT) OXFL =(100.-MIX(IST))/MIX(IST)                           MAIN 239
      IF(.NOT.ERATIO)  GO TO 333                                        MAIN 240
      EQRAT = MIX(IST)                                                  MAIN 241
      IF(EQRAT.EQ.1.)  EQRAT = 1.0C00045                                MAIN 242
      OXFL = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))           MAIN 243
  333 OXF(IST) = OXFL                                                   MAIN 244
      NOF = IST                                                         MAIN 245
  625 CONTINUE                                                          MAIN 246
  745 IF (.NOT.ICNS) GO TO 746                                          MAIN 247
      IF(LLMT(NLM).EQ.IE)  GO TO 746                                    MAIN 248
      NLM = NLM+1                                                       MAIN 249
      IF(LLMT(NLM).NE.IE)  NEWR=.TRUE.                                  MAIN 250
      REWIND 4                                                          MAIN 251
      LLMT(NLM) = IE                                                    MAIN 252
      BOP(NLM,1) = 0.                                                   MAIN 253
      BOP(NLM,2) = 0.                                                   MAIN 254
      GO TO 748                                                         MAIN 255
  746 IF(LLMT(NLM).NE.IE)  GO TO 748                                    MAIN 256
      DO 747  J=1,NS                                                    MAIN 257
      IF(A(NLM,J).NE.0.)  IUSE(J)=-10000                                MAIN 258
  747 CONTINUE                                                          MAIN 259
      NLM = NLM-1                                                       MAIN 260
  748 IF(NEWR)  CALL SEARCH                                             MAIN 261
      IF(NS.EQ.0)  GO TO 1                                              MAIN 262
C                                                                       MAIN 263
C     INITIAL ESTIMATES                                                 MAIN 264
C                                                                       MAIN 265
      SO = SO/R                                                         MAIN 266
      ENN = .1                                                          MAIN 267
      ENNL = -2.3025851                                                 MAIN 268
      SUMN = ENN                                                        MAIN 269
      XI = NS - NC                                                      MAIN 270
```

```
      XI = ENN/XI                                                       MAIN 271
      XLN = ALOG(XI)                                                    MAIN 272
      DO 432 J=1,NS                                                     MAIN 273
      IF(IUSE(J).GT.0)  IUSE(J)=-IUSE(J)                                MAIN 274
      IF(IUSE(J).EQ.-10000.AND.IONS)  IUSE(J) = 0                       MAIN 275
      EN(J,1) = 0.                                                      MAIN 276
      ENLN(J) = 0.                                                      MAIN 277
      IF (IUSE(J).NE.0)  GO TO 432                                      MAIN 278
      EN(J,1) = XI                                                      MAIN 279
      ENLN(J) = XLN                                                     MAIN 280
  432 CONTINUE                                                          MAIN 281
      IQ1 = NLM+1                                                       MAIN 282
      IF (NC.EQ.0.OR.NSERT.EQ.0) GO TO 790                              MAIN 283
      DO 302 I=1,NSERT                                                  MAIN 284
      INC = 0                                                           MAIN 285
      DO 301 J=1,NS                                                     MAIN 286
      IF(IUSE(J).EQ.0) GO TO 301                                        MAIN 287
      INC = INC+1                                                       MAIN 288
      IF(SUB(J,1).NE.ENSERT(1,I)) GO TO 301                             MAIN 289
      IF(SUB(J,2).NE.ENSERT(2,I)) GO TO 301                             MAIN 290
      IF(SUB(J,3).NE.ENSERT(3,I)) GO TO 301                             MAIN 291
      IF(T(1).EQ.0.)  GO TO 295                                         MAIN 292
      IF(T(1).LT.TEMP(INC,1).OR.T(1).GT.TEMP(INC,2))  GO TO 301         MAIN 293
  295 IQ1 = IQ1+1                                                       MAIN 294
      IUSE(J)= -IUSE(J)                                                 MAIN 295
      GO TO 302                                                         MAIN 296
  301 CONTINUE                                                          MAIN 297
  302 CONTINUE                                                          MAIN 298
      NSERT = 0                                                         MAIN 299
  790 CONTINUE                                                          MAIN 300
      IF(.NOT.TP.AND..NOT.HP.AND..NOT.SP)  GO TO 791                    MAIN 301
      CALL THERMP                                                       MAIN 302
      GO TO 800                                                         MAIN 303
  791 CONTINUE                                                          MAIN 304
      IF(DETN) CALL DETON                                               MAIN 305
      IF(RKT) CALL ROCKET                                               MAIN 306
      IF(SHOCK)  CALL SHCK                                              MAIN 307
  800 RETURN                                                            MAIN 308
      END                                                               MAIN 309
```

```
C
      SUBROUTINE REACT                                                  REAC   1
C                                                                       REAC   2
      LOGICAL HP,SP,TP,CONVG,NEWR,IONS,MOLES,EQL,FROZ,VOL               REAC   3
C                                                                       REAC   4
      DIMENSION ANAME(15,5),V(10)                                       REAC   5
C                                                                       REAC   6
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),REAC   7
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      REAC   8
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         REAC   9
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FCX(15),DENS(15),REAC  10
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      REAC  11
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   REAC  12
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, REAC  13
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, REAC  14
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            REAC  15
C                                                                       REAC  16
      EQUIVALENCE (NAME,ANAME),(NLM,L),(BLANK,LANK)                     REAC  17
```

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C                                                                       REAC  18
      DATA MOL/1HM/,OX/1HO/,LANK/1H /,IZERO/2H00/,ZERO/1H0/             REAC  19
C                                                                       REAC  20
      DO 10 K=1,2                                                       REAC  21
      WP(K)=0.                                                          REAC  22
      HPP(K)=0.                                                         REAC  23
      RM(K)=0.                                                          REAC  24
      VPLS(K)=0.                                                        REAC  25
      VMIN(K)=0.                                                        REAC  26
      AM(K)=0.                                                          REAC  27
      DO 8 J=1,10                                                       REAC  28
      LLMT(J)=0                                                         REAC  29
      BOP(J,K)=0.                                                       REAC  30
    8 CONTINUE                                                          REAC  31
   10 CONTINUE                                                          REAC  32
      NFUEL = 0                                                         REAC  33
      N=1                                                               REAC  34
      L=1                                                               REAC  35
C                                                                       REAC  36
C     READ AND WRITE REACTANT CARDS                                     REAC  37
C                                                                       REAC  38
   20 READ(5,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),      REAC  39
     1 FAZ(N),RTEMP(N),FOX(N),DENS(N)                                   REAC  40
   21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F8.5,A1,F8.5)                   REAC  41
      IF(NAME(N,1).EQ.LANK) GO TO 200                                   REAC  42
      IF(L.EQ.0)GO TO 20                                                REAC  43
      WRITE (6,31)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),    REAC  44
     1 FAZ(N),RTEMP(N),FOX(N),DENS(N)                                   REAC  45
   31 FORMAT(1X,5(A2,1X,F7.4,2X),F8.4,2X,A1,F11.2,2X,A1,2X,F8.3,2X,     REAC  46
     1 A1,3X,F8.5)                                                      REAC  47
   35 IF(MOLE.EQ.MOL) MOLES=.TRUE.                                      REAC  48
C                                                                       REAC  49
C     IF OXIDANT, K=1                                                   REAC  50
C     IF FUEL, K=2                                                      REAC  51
C                                                                       REAC  52
      IF(FOX(N).EQ.ZERO)  FOX(N)=OX                                     REAC  53
      K = 1                                                             REAC  54
      IF(FOX(N).EQ.OX)  GO TO 37                                        REAC  55
      K = 2                                                             REAC  56
      NFUEL = NFUEL+1                                                   REAC  57
   37 DO 38  J=1,15                                                     REAC  58
      DATA(J) = 0.                                                      REAC  59
   38 CONTINUE                                                          REAC  60
      RM=0.                                                             REAC  61
C                                                                       REAC  62
C     STORE ATOMIC SYMBOLS IN LLMT ARRAY.                               REAC  63
C     CALCULATE MOLECULAR WEIGHT.                                       REAC  64
C     TEMPORARILY STORE ATOMIC VALENCE IN V.                            REAC  65
C                                                                       REAC  66
      DO 100 JJ=1,5                                                     REAC  67
      IF(ANUM(N,JJ).EQ.0.)GO TO 101                                     REAC  68
      IF(ANAME(N,JJ).EQ.ZERO)  ANAME(N,JJ)=OX                           REAC  69
      DO 41 J=1,10                                                      REAC  70
      NJ = J                                                            REAC  71
      IF(LLMT(J).EQ.0) GO TO 45                                         REAC  72
      IF(NAME(N,JJ).EQ.LLMT(J))GO TO 46                                 REAC  73
   41 CONTINUE                                                          REAC  74
   45 L = NJ                                                            REAC  75
      LLMT(J)=NAME(N,JJ)                                                REAC  76
   46 DO 48 KK=1,101                                                    REAC  77
      IF(ATOM(1,KK).EQ.ANAME(N,JJ))GO TO 50                             REAC  78
   48 CONTINUE                                                          REAC  79
      L=0                                                               REAC  80
      GO TO 20                                                          REAC  81
   50 RM=RM+ANUM(N,JJ)*ATOM(2,KK)                                       REAC  82
```

```
      V$J)=ATOM(3,KK)                                                    REAC  83
      DATA(J)=ANUM(N,JJ)                                                 REAC  84
  100 CONTINUE                                                           REAC  85
C                                                                        REAC  86
C     ADD CONTRIBUTIONS TO WP(K), HPP(K), AM(K), BOP(I,K) AND RH(K)      REAC  87
C                                                                        REAC  88
  101 PCWT=PECWT(N)                                                      REAC  89
      IF(MOLES) PCWT=PCWT*RM                                             REAC  90
      WP(K)=WP(K) + PCWT                                                 REAC  91
      EM = ENTH(N)                                                       REAC  92
      IF(NAME(N,5).NE.IZERO)HPP(K)=HPP(K)+EM*PCWT/(RM*R)                 REAC  93
      AM(K)=AM(K)+PCWT/RM                                                REAC  94
      DO 110  J=1,L                                                      REAC  95
      BOP(J,K)=DATA(J)*PCWT/RM +BOP(J,K)                                 REAC  96
  110 CONTINUE                                                           REAC  97
      IF(DENS(N).NE.0.)GO TO 115                                         REAC  98
      GO TO 117                                                          REAC  99
  115 RH(K)=RH(K)+PCWT/DENS(N)                                           REAC 100
  117 RMW(N) = RM                                                        REAC 101
      N = N+1                                                            REAC 102
      IF(N.NE.16) GO TO 20                                               REAC 103
  200 NREAC =N-1                                                         REAC 104
      IF(NFUEL.GT.0)  GO TO 210                                          REAC 105
C                                                                        REAC 106
C     100 PERCENT OXIDANT, CALL REACTANTS FUEL                           REAC 107
C                                                                        REAC 108
      DO 205  N=1,NREAC                                                  REAC 109
      FOX(N) = BLANK                                                     REAC 110
  205 CONTINUE                                                           REAC 111
      RH(2) = RH(1)                                                      REAC 112
      RH(1) = 0.                                                         REAC 113
      WP(2) = WP(1)                                                      REAC 114
      WP(1) = 0.                                                         REAC 115
      HPP(2) = HPP(1)                                                    REAC 116
      AM(2) = AM(1)                                                      REAC 117
      AM(1) = 0.                                                         REAC 118
      DO 208  J=1,L                                                      REAC 119
      BOP(J,2) = BOP(J,1)                                                REAC 120
  208 CONTINUE                                                           REAC 121
  210 IF(L.EQ.0)  GO TO 1000                                             REAC 122
C                                                                        REAC 123
C     NORMALIZE HPP(K),AM(K),BOP(I,K), AND PECWT(N).                     REAC 124
C     CALCULATE RH(K), V+(K), AND V-(K)                                  REAC 125
C                                                                        REAC 126
      DO 220 K=1,2                                                       REAC 127
      IF(WP(K).EQ.0.)GO TO 220                                           REAC 128
      HPP(K)=HPP(K)/WP(K)                                                REAC 129
      AM(K) = WP(K)/AM(K)                                                REAC 130
      IF(RH(K).NE.0.)RH(K)=WP(K)/RH(K)                                   REAC 131
      DO 215 J=1,L                                                       REAC 132
      BOP(J,K)=BOP(J,K)/WP(K)                                            REAC 133
      IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)                       REAC 134
      IF(V(J).GT.0.)VPLS(K)=VPLS(K)+BOP(J,K)*V(J)                        REAC 135
  215 CONTINUE                                                           REAC 136
      IF(MOLES) GO TO 220                                                REAC 137
      DO 218 N=1,NREAC                                                   REAC 138
      IF(FOX(N).EQ.OX.AND.K.EQ.2)  GO TO 218                             REAC 139
      IF(FOX(N).NE.OX.AND.K.EQ.1)  GO TO 218                             REAC 140
      PECWT(N) = PECWT(N)/WP(K)                                          REAC 141
  218 CONTINUE                                                           REAC 142
  220 CONTINUE                                                           REAC 143
      NEWR=.TRUE.                                                        REAC 144
C                                                                        REAC 145
C  ARE ELEMENTS SAME AS FOR  LAST SET OF REACTANTS, IF SO, NEWR=.FALSE.  REAC 146
```

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                                                                      REAC 147
      IF(NLM.NE.NLS)  GO TO 226                                       REAC 148
      IF(NOMIT.NE.0)  GO TO 226                                       REAC 149
      DO 224 I=1,NLS                                                  REAC 150
      DO 222  J=1,NLM                                                 REAC 151
      IF(LLMT(J).NE.LLMTS(I))  GO TO 222                              REAC 152
      SBOP(I,1) = BOP(J,1)                                            REAC 153
      SBOP(I,2) = BOP(J,2)                                            REAC 154
      GO TO 224                                                       REAC 155
  222 CONTINUE                                                        REAC 156
      GO TO 226                                                       REAC 157
  224 CONTINUE                                                        REAC 158
      NEWR = .FALSE.                                                  REAC 159
      DO 225  I=1,NLM                                                 REAC 160
      LLMT(I) = LLMTS(I)                                              REAC 161
      BOP(I,1)  = SBOP(I,1)                                           REAC 162
      BOP(I,2)  = SBOP(I,2)                                           REAC 163
  225 CONTINUE                                                        REAC 164
      GO TO 229                                                       REAC 165
C                                                                     REAC 166
C                                                                     REAC 167
  226 NLS = NLM                                                       REAC 168
      NOMIT = 0                                                       REAC 169
      REWIND 4                                                        REAC 170
      DO 228 I=1,NLM                                                  REAC 171
      LLMTS(I) = LLMT(I)                                              REAC 172
  228 CONTINUE                                                        REAC 173
  229 DO 230  N=1,NREAC                                               REAC 174
      IF (CENS(N).NE.0.) GO TO 230                                    REAC 175
      RH(2) = 0.                                                      REAC 176
      RH (1) = 0.                                                     REAC 177
      GO TO 1000                                                      REAC 178
  230 CONTINUE                                                        REAC 179
 1000 RETURN                                                          REAC 180
      END                                                             REAC 181
```

```
C
      SUBROUTINE SEARCH                                               SRCH   1
C                                                                     SRCH   2
C  SEARCH TAPE FOR THERMO DATA AND TRANSPORT CROSS SECTIONS OF SPECIES SRCH   3
C                    TO BE CONSIDERED                                 SRCH   4
C                                                                     SRCH   5
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR    SRCH   6
C     IBM 360 MACHINES ONLY                                           SRCH   7
C                                                                     SRCH   8
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                         SRCH   9
C                                                                     SRCH  10
      INTEGER SUB,OMIT,END,TOOBIG                                     SRCH  11
      INTEGER SPECE                                                   SRCH  12
C                                                                     SRCH  13
      LOGICAL NEWR,OTTO,TRNSPT                                        SRCH  14
C                                                                     SRCH  15
      DIMENSION DATE(2,3),NT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50)    SRCH  16
      DIMENSION SPECE(2,3),TEMPR(20),TABLS(20,3)                      SRCH  17
C                                                                     SRCH  18
      COMMON   SPECE , TEMPR , TABLS                                  SRCH  19
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), SRCH  20
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)  SRCH  21
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),SRCH  22
```

```
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),          SRCH  23
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),            SRCH  24
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),   SRCH  25
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)         SRCH  26
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,      SRCH  27
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,    SRCH  28
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,    SRCH  29
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT               SRCH  30
C                                                                          SRCH  31
      EQUIVALENCE (DATE,EN),(OMIT,ENLN),(ENDD,END),(TOOBIG,ENLN)           SRCH  32
C                                                                          SRCH  33
      DATA  GAS/1HG/,END/3HEND/,ND/4HLAST/                                 SRCH  34
C                                                                          SRCH  35
C                                                                          SRCH  36
C                   SEARCH FOR THERMO DATA                                 SRCH  37
C                                                                          SRCH  38
      I2B = 0                                                              SRCH  39
      NC= C                                                                SRCH  40
      IX= C                                                                SRCH  41
C                                                                          SRCH  42
C  CHECK DIMENSION FOR NUMBER OF SPECIES, CLEAR A(I,J)                     SRCH  43
C                                                                          SRCH  44
      SUB(1,1) = END                                                       SRCH  45
      DO 3  I=1,1000                                                       SRCH  46
      IF(A(1,I).EQ.ENDD)  GO TO 4                                          SRCH  47
      DO 3 J=1,NLM                                                         SRCH  48
      A(J,I) = 0.                                                          SRCH  49
    3 CONTINUE                                                             SRCH  50
    4 MAXNS = I-1                                                          SRCH  51
C                                                                          SRCH  52
C  READ TEMPERATURE RANGES FOR COEFFICIENTS OF GASEOUS SPECIES.            SRCH  53
C                                                                          SRCH  54
      READ(4,5)  TLOW,TMID,THIGH                                           SRCH  55
    5 FORMAT (3F10.3)                                                      SRCH  56
      NS = 1                                                               SRCH  57
C                                                                          SRCH  58
C  BEGIN LOOP FOR READING SPECIES DATA FROM TAPE.                          SRCH  59
C                                                                          SRCH  60
    7 READ (4,10)  (NAM(I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J),      SRCH  61
     1 J=1,4),PHAZ,T1,T2                                                   SRCH  62
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                              SRCH  63
      IF(NAM(1).EQ.END)  GO TO 171                                         SRCH  64
      READ (4,20)  ((COEF(I,J,NS),J=1,7),I=1,2)                            SRCH  65
   20 FORMAT (5E15.8)                                                      SRCH  66
      IF(NOMIT.EQ.0) GO TO 810                                             SRCH  67
      DO 805 I=1,NOMIT                                                     SRCH  68
      DO 804 J=1,3                                                         SRCH  69
      IF(OMIT(J,I).NE.NAM(J)) GO TO 805                                    SRCH  70
  804 CONTINUE                                                             SRCH  71
      GO TO 7                                                              SRCH  72
  805 CONTINUE                                                             SRCH  73
  810 DO 820 K=1,4                                                         SRCH  74
      IF(B(K).EQ.0.) GO TO 825                                             SRCH  75
      DO 168 I=1,NLM                                                       SRCH  76
      IF(LLMT(I).EQ.MT(K)) GO TO 820                                       SRCH  77
  168 CONTINUE                                                             SRCH  78
      IF(NS.GT.MAXNS)  GO TO 7                                             SRCH  79
      DO 819 J=1,NLM                                                       SRCH  80
  819 A(J,NS) = 0.                                                         SRCH  81
      GO TO 7                                                              SRCH  82
  820 IF(NS.LE.MAXNS)  A(I,NS) = B(K)                                      SRCH  83
  825 IF(NS.LE.MAXNS)  GO TO 828                                           SRCH  84
      I2B = I2B+1                                                          SRCH  85
      DO 826  I=1,3                                                        SRCH  86
```

```
  826 TOOBIG(I,I2B) = NAM(I)                                              SRCH  87
      GO TO 7                                                             SRCH  88
  828 DO 829  I=1,3                                                       SRCH  89
  829 SUB(NS,I) = NAM(I)                                                  SRCH  90
      IUSE(NS) = 0                                                        SRCH  91
      IF(PHAZ.EQ.GAS) GO TO 170                                           SRCH  92
C                                                                         SRCH  93
C  CONDENSED SPECIES                                                      SRCH  94
C                                                                         SRCH  95
      NC= NC+1                                                            SRCH  96
      TEMP(NC,1)= T1                                                      SRCH  97
      TEMP(NC,2)= T2                                                      SRCH  98
      IX= IX+1                                                            SRCH  99
      IF(NS.EQ.1.OR.IUSE(NS-1).EQ.0)  GO TO 145                           SRCH 100
      DO 830 I=1,NLM                                                      SRCH 101
      IF(A(I,NS).NE.A(I,NS-1)) GO TO 145                                  SRCH 102
  830 CONTINUE                                                            SRCH 103
      IX= IX-1                                                            SRCH 104
  145 IUSE(NS)= -IX                                                       SRCH 105
  170 NS= NS+1                                                            SRCH 106
      GO TO 7                                                             SRCH 107
C                                                                         SRCH 108
C  END CARD HAS BEEN READ.                                                SRCH 109
C                                                                         SRCH 110
  171 NS= NS-1                                                            SRCH 111
      NEWR= .FALSE.                                                       SRCH 112
      WRITE(6,172)                                                        SRCH 113
  172 FORMAT(42HOSPECIES BEING CONSIDERED IN THIS SYSTEM    )             SRCH 114
      DO 174 I=1,NS,5                                                     SRCH 115
      I5= I+4                                                             SRCH 116
      IF(NS.LT.I5) I5=NS                                                  SRCH 117
  174 WRITE (6,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),       SRCH 118
     1 J=I,I5)                                                            SRCH 119
  176 FORMAT(5(5X,2A3,2X,3A4))                                            SRCH 120
      IF(I2B.GT.0)  GO TO 870                                             SRCH 121
      GO TO 16                                                            SRCH 122
  870 WRITE(6,871)  I2B                                                   SRCH 123
  871 FORMAT(35HOINSUFFICIENT STORAGE FOR FOLLOWING,I3,8H SPECIES)        SRCH 124
      WRITE(6,880)(TOOBIG(1,J),TOOBIG(2,J),TOOBIG(3,J),J=1,I2B)          SRCH 125
  880 FORMAT(8(3X,3A4))                                                   SRCH 126
      NS = 0                                                              SRCH 127
C                                                                         SRCH 128
C                    SEARCH FOR TRANSPORT CROSS SECTIONS                  SRCH 129
C                                                                         SRCH 130
   16 NK = 1                                                              SRCH 131
   13 READ(4) ((SPECE(I,L),L=1,3),I=1,2),NTP,NTB,ROTN                     SRCH 132
      IF(SPECE(1,1).EQ.ND) GO TO 21                                       SRCH 133
      K=1                                                                 SRCH 134
      DO 25 J=1,NS                                                        SRCH 135
      DO 24 I=1,3                                                         SRCH 136
   24 IF(SPECE(K,I).NE.SUB(J,I)) GO TO 25                                 SRCH 137
      GO TO 6                                                             SRCH 138
   25 CONTINUE                                                            SRCH 139
      GO TO 13                                                            SRCH 140
    6 K=2                                                                 SRCH 141
      DO 8 JJ=1,NS                                                        SRCH 142
      DO 27 II=1,3                                                        SRCH 143
   27 IF(SPECE(K,II).NE.SUB(JJ,II)) GO TO 8                               SRCH 144
      GO TO 21                                                            SRCH 145
    8 CONTINUE                                                            SRCH 146
      GO TO 13                                                            SRCH 147
   21 WRITE(3) ((SPECE(I,L),L=1,3),I=1,2),NTP,NTB,ROTN                    SRCH 148
      IF(SPECE(1,1).EQ.ND) GO TO 17                                       SRCH 149
      READ(4) (TEMPR(I),(TABLS(I,L),L=1,3),I=1,NTP)                       SRCH 150
      WRITE(3) (TEMPR(I),(TABLS(I,L), L=1,3),I=1,NTP)                     SRCH 151
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      NK=NK+1                                                          SRCH 152
      GO TO 13                                                         SRCH 153
   17 CONTINUE                                                         SRCH 154
      REWIND 3                                                         SRCH 155
      RETURN                                                           SRCH 156
      END                                                              SRCH 157
C
      SUBROUTINE HCALC                                                 HCAL   1
C                                                                      HCAL   2
C     CALCULATE PROPERTIES FOR TOTAL REACTANT USING THERMO DATA FOR    HCAL   3
C     ONE OR MORE REACTANTS.                                           HCAL   4
C                                                                      HCAL   5
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR     HCAL   6
C     IBM 360 MACHINES ONLY                                            HCAL   7
C                                                                      HCAL   8
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                HCAL   9
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                          HCAL  10
C                                                                      HCAL  11
      LOGICAL MOLES,VOL,SHOCK,CALCH                                    HCAL  12
C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                HCAL  13
      DIMENSION NUM(15,5)                                              HCAL  14
C                                                                      HCAL  15
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),    HCAL  16
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13), HCAL  17
     2 VLM(13),TOTN(13)                                                HCAL  18
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), HCAL  19
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)  HCAL  20
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),HCAL  21
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      HCAL  22
     2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),          HCAL  23
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),HCAL  24
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      HCAL  25
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   HCAL  26
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, HCAL  27
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, HCAL  28
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            HCAL  29
C                                                                      HCAL  30
      EQUIVALENCE (ANUM,NUM),(L,NLM),(J,JS1)                           HCAL  31
      EQUIVALENCE (AM1,DATA(20)),(CPR1,DATA(21))                       HCAL  32
C                                                                      HCAL  33
      DATA AG/1HG/,IZERO/2H00/,OX/1HO/,BLK/1H /                        HCAL  34
C                                                                      HCAL  35
      TSAVE = TT                                                       HCAL  36
C                                                                      HCAL  37
C     CALCUALTE MOLECULAR WEIGHT OF TOTAL REACTANT, AM1.               HCAL  38
C                                                                      HCAL  39
      IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GO TO4                      HCAL  40
      AM1= AM(2)                                                       HCAL  41
      IF (AM(2).EQ.0.0) AM1= AM(1)                                     HCAL  42
      GO TO 9                                                          HCAL  43
    4 AM1=(OF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2))                         HCAL  44
    9 TM = 0.                                                          HCAL  45
      IF(PP.GT.0.) TM = ALOG(PP*AM1)                                   HCAL  46
      SSUM(NPT) = 0.                                                   HCAL  47
      HPP(1) = 0.                                                      HCAL  48
      HPP(2) = 0.                                                      HCAL  49
      HSUBO = 0.                                                       HCAL  50
```

```
      CPR1 = 0.                                                          HCAL  51
      ANN = (1.+CF)                                                      HCAL  52
C                                                                        HCAL  53
C     LOOP ON REACTANTS.                                                 HCAL  54
C     IF OXIDANT, K=1                                                    HCAL  55
C     IF FUEL, K=2                                                       HCAL  56
C                                                                        HCAL  57
      DO 900 N=1,NREAC                                                   HCAL  58
      K=2                                                                HCAL  59
      IF(FOX(N).EQ.OX)K=1                                                HCAL  60
      IF(NAME(N,5).NE.IZERO)  GO TO 90                                   HCAL  61
      IF(.NOT.CALCH.AND.TT.NE.0.)  GO TO 15                              HCAL  62
      TT = RTEMP(N)                                                      HCAL  63
C                                                                        HCAL  64
C  IS TT IN RANGE                                                        HCAL  65
C                                                                        HCAL  66
   15 IF(SHOCK)  GO TO 16                                                HCAL  67
      IF(TT.LT.(TLOW/1.2).OR.TT.GT.(THIGH*1.2))  GO TO 75                HCAL  68
   16 J = NUM(N,5)                                                       HCAL  69
      IF (J.NE.0)  GO TO 90                                              HCAL  70
      DO 10 J=1,L                                                        HCAL  71
      DATA(J)=0.                                                         HCAL  72
   10 CONTINUE                                                           HCAL  73
C                                                                        HCAL  74
C     TEMPORARILY STORE STOICHIOMETRIC COEFFICIENTS IN DATA ARRAY.       HCAL  75
C                                                                        HCAL  76
      DO 40 I=1,4                                                        HCAL  77
      IF(ANUM(N,I).EQ.0.)GO TO 50                                        HCAL  78
      DO 20 J=1,L                                                        HCAL  79
      IF(LLMT(J).EQ.NAME(N,I))GO TO 30                                   HCAL  80
   20 CONTINUE                                                           HCAL  81
   30 DATA(J)=ANUM(N,I)                                                  HCAL  82
   40 CONTINUE                                                           HCAL  83
   50 IS=0                                                               HCAL  84
C                                                                        HCAL  85
C     SEARCH FOR REACTANT IN THERMO SPECIES.  STORE INDEX IN NUM(N,5).   HCAL  86
C                                                                        HCAL  87
      DO 70 J=1,NS                                                       HCAL  88
      IF(IUSE(J).EQ.0)GO TO 55                                           HCAL  89
      IS = IS+1                                                          HCAL  90
      IF(FAZ(N).EQ.AG)GO TO 70                                           HCAL  91
      IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH)  GO TO 70             HCAL  92
      IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW)  GO TO 70              HCAL  93
      GO TO 56                                                           HCAL  94
   55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK)  GO TO 70                       HCAL  95
   56 DO 60 I=1,L                                                        HCAL  96
      IF(A(I,J).NE.DATA(I))  GO TO 70                                    HCAL  97
   60 CONTINUE                                                           HCAL  98
      NUM(N,5) = J                                                       HCAL  99
      GO TO 90                                                           HCAL 100
   70 CONTINUE                                                           HCAL 101
      GO TO 80                                                           HCAL 102
C                                                                        HCAL 103
C     CALCULATE EN FOR REACTANT AND CALL CPHS TO CALCULATE PROPERTIES.   HCAL 104
C                                                                        HCAL 105
   90 IF (MOLES)   ENJ = PECWT(N)/WP(K)                                  HCAL 106
      IF (.NOT.MOLES)   ENJ = PECWT(N)/RMW(N)                            HCAL 107
      ENJ = ENJ/ANN                                                      HCAL 108
      IF(K.EQ.1)  ENJ = ENJ*OF                                           HCAL 109
      IF(NAME(N,5).NE.IZERO)GO TO 500                                    HCAL 110
      NSS = NS                                                           HCAL 111
      NS = J                                                             HCAL 112
      TLN = ALOG(TT)                                                     HCAL 113
      IF(.NOT.CALCH)  EN(J,NPT) = ENJ                                    HCAL 114
      CALL CPHS                                                          HCAL 115
```

```
      NS = NSS                                                          HCAL 116
      IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.                  HCAL 117
      RTEMP(N) = TT                                                     HCAL 118
      IF(VOL) HO(J)=HO(J)-1.                                            HCAL 119
      ENTH(N) = HO(J)*R*TT                                              HCAL 120
C                                                                       HCAL 121
C     ADD CONTRIBUTION TO CP, H, AND S OF TOTAL REACTANT.               HCAL 122
C                                                                       HCAL 123
      CPR1 = CPR1 + CPSUM                                               HCAL 124
      SSUM(NPT) = SSUM(NPT) + ENJ * (S(J)-ALOG(ENJ)-TM)                 HCAL 125
  500 ER = ENTH(N)*ENJ/R                                                HCAL 126
      HSUBO = HSUBO+ER                                                  HCAL 127
      HPP(K) = HPP(K)+ER                                                HCAL 128
  900 CONTINUE                                                          HCAL 129
      IF(TSAVE.NE.0.)  TT=TSAVE                                         HCAL 130
      GO TO 1000                                                        HCAL 131
   75 WRITE(6,76)                                                       HCAL 132
   76 FORMAT(50HOREACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA )     HCAL 133
      TT = 0.                                                           HCAL 134
      GO TO 1000                                                        HCAL 135
   80 WRITE(6,85) N                                                     HCAL 136
   85 FORMAT(9HOREACTANT,I2,22H IS NOT IN THERMO DATA )                 HCAL 137
      TT = 0.                                                           HCAL 138
 1000 RETURN                                                            HCAL 139
      END                                                               HCAL 140
```

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C
      SUBROUTINE SAVE                                                   SAVE   1
C                                                                       SAVE   2
C  SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES  SAVE   3
C                                                                       SAVE   4
C                                                                       SAVE   5
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      SAVE   6
C     IBM 360 MACHINES ONLY                                             SAVE   7
C                                                                       SAVE   8
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           SAVE   9
C                                                                       SAVE  10
      LOGICAL VOL,CALCH,IONS,SHOCK                                      SAVE  11
C                                                                       SAVE  12
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), SAVE  13
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   SAVE  14
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),SAVE  15
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      SAVE  16
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         SAVE  17
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),SAVE  18
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      SAVE  19
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   SAVE  20
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, SAVE  21
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, SAVE  22
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            SAVE  23
      COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,    SAVE  24
     1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,            SAVE  25
     2 FIRSTP,FIRSTV                                                    SAVE  26
C                                                                       SAVE  27
      DATA IE/1HE/                                                      SAVE  28
C                                                                       SAVE  29
      IF(ISV)100,10,200                                                 SAVE  30
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C                                                                       SAVE  31
C  NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITICNS FOR THIS T SAVE  32
C                                                                       SAVE  33
   10 IQ1 = IQSAVE                                                      SAVE  34
      JSOL = JSOLS                                                      SAVE  35
      JLIQ = JLIQS                                                      SAVE  36
      ENN = ENSAVE                                                      SAVE  37
      ENNL = ENLSAV                                                     SAVE  38
      LL1 = NLM                                                         SAVE  39
      DC 5C J = 1,NS                                                    SAVE  40
      IF(.NCT.IONS)  GO TO 15                                           SAVE  41
      IF(LLMT(NLM).EQ.LSAVE)  GO TC 15                                  SAVE  42
      IF(LLMT(NLM).EQ.IE)  GO TO 13                                     SAVE  43
      IF(IUSE(J).NE.-10000)  GO TO 15                                   SAVE  44
      IUSE(J) = 0                                                       SAVE  45
      LL1  = NLM+1                                                      SAVE  46
      GO TC 20                                                          SAVE  47
   13 IF(SLN(J).NE.0..CR.IUSE(J).NE.0)  GO TO 15                        SAVE  48
      LL1 = NLM-1                                                       SAVE  49
      IUSE(J) = -10000                                                  SAVE  50
      GC TC 50                                                          SAVE  51
   15 IF (IUSE(J).EQ.0) GO TO 20                                        SAVE  52
      EN (J,NPT) = SLN(J)                                               SAVE  53
      IF(IUSE(J).GT.0) IUSE(J) = -IUSE(J)                               SAVE  54
      IF (EN(J,NPT).NE.0.)IUSE(J) = -IUSE(J)                            SAVE  55
      GC TC 50                                                          SAVE  56
   20 EN(J,NPT) = C.                                                    SAVE  57
      ENLN(J) = SLN(J)                                                  SAVE  58
      IF ((ENLN(J)-ENNL + 18.5).LE.0.) GO TO 50                         SAVE  59
      EN(J,NPT) = 2.718281828459**ENLN(J)                               SAVE  60
   50 CONTINUE                                                          SAVE  61
      NLM = LL1                                                         SAVE  62
      GC TO 1000                                                        SAVE  63
C                                                                       SAVE  64
C  FIRST T--SAVE COMPOSITICNS FOR FUTURE POINTS WITH THIS T             SAVE  65
C                                                                       SAVE  66
  100 ISV = -ISV                                                        SAVE  67
      JSOLS = JSOL                                                      SAVE  68
      JLIQS = JLIQ                                                      SAVE  69
      IQSAVE = IQ1                                                      SAVE  70
      ENSAVE = ENN                                                      SAVE  71
      ENLSAV = ENNL                                                     SAVE  72
      LSAVE = LLMT(NLM)                                                 SAVE  73
      DC 150 J = 1,NS                                                   SAVE  74
      SLN(J) = ENLN(J)                                                  SAVE  75
      IF(IUSE(J).NE.0)  SLN(J)=EN(J,ISV)                                SAVE  76
  150 CONTINUE                                                          SAVE  77
C                                                                       SAVE  78
C  USE CCMPCSITICNS FROM PREVIOUS POINT                                 SAVE  79
C                                                                       SAVE  80
  200 DO 300 J = 1,NS                                                   SAVE  81
      EN(J,NPT) = EN(J,ISV)                                             SAVE  82
  300 CONTINUE                                                          SAVE  83
 1000 RETURN                                                            SAVE  84
C                                                                       SAVE  85
C  CALCULATE NEW VALUES OF BO AND HSUBO FOR NEW OF RATIC                SAVE  86
C                                                                       SAVE  87
      ENTRY NEWOF                                                       SAVE  88
C                                                                       SAVE  89
C                                                                       SAVE  90
      WRITE(6,730) OF                                                   SAVE  91
  730 FORMAT(6HOOF = ,F10.6)                                            SAVE  92
      EQRAT = 0.                                                        SAVE  93
      SUM = OF + 1.                                                     SAVE  94
      V1 = (OF*VPLS(1)+VPLS(2))/SUM                                     SAVE  95
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      V2 = (OF*VMIN(1)+VMIN(2))/SUM                                          SAVE  96
      IF(V2.NE.0.)  EQRAT=ABS(V1/V2)                                         SAVE  97
      IF  (RH(1) .NE. 0. .AND. RH(2) .NE. 0.) GO TO 744                      SAVE  98
      RHOP = RH(2)                                                           SAVE  99
      IF (RHOP .EQ. 0.) RHOP = RH(1)                                         SAVE 100
      GO TO 745                                                              SAVE 101
  744 RHOP =  (OF+1.)*RH(1)*RH(2)/(RH(1)+OF*RH(2))                           SAVE 102
  745 DO 747 I=1,NLM                                                         SAVE 103
      BO(I) = (OF*BOP(I,1)+BOP(I,2))/SUM                                     SAVE 104
  747 CONTINUE                                                               SAVE 105
      NPT = 1                                                                SAVE 106
      IF(.NOT.CALCH)  GO TO 750                                              SAVE 107
      CALL HCALC                                                             SAVE 108
      IF(TT.EQ.0.)  RETURN                                                   SAVE 109
      CALCH = .FALSE.                                                        SAVE 110
      IF(OF.NE.0.)  HPP(1)=SUM*HPP(1)/OF                                     SAVE 111
      HPP(2) = SUM*HPP(2)                                                    SAVE 112
      GO TO 760                                                              SAVE 113
  750 HSUBO=  (OF*HPP(1) + HPP(2))/SUM                                       SAVE 114
  760 IC = 0                                                                 SAVE 115
      JSOL = 0                                                               SAVE 116
      JLIQ = 0                                                               SAVE 117
      WRITE (6,770)                                                          SAVE 118
  770 FORMAT(1H ,25X,14HEFFECTIVE FUEL,10X,17HEFFECTIVE OXIDANT,12X,7HMI SAVE 119
     1XTURE )                                                                SAVE 120
      IF(VOL)  WRITE(6,772)                                                  SAVE 121
      IF(.NOT.VOL)  WRITE(6,774)                                             SAVE 122
  772 FORMAT(16H INTERNAL ENERGY,14X,6HHPP(2),19X,6HHPP(1),19X,5HHSUBO )SAVE 123
  774 FORMAT(9H ENTHALPY,21X,6HHPP(2),19X,6HHPP(1),19X,5HHSUBO )         SAVE 124
      WRITE(6,776)  HPP(2),HPP(1),HSUBO                                      SAVE 125
  776 FORMAT(19H (KG-MOL)(DEG K)/KG,E21.8,2E25.8 )                           SAVE 126
      WRITE(6,778)                                                           SAVE 127
  778 FORMAT(12HOKG-ATOMS/KG,17X,8HBOP(I,2),17X,8HBOP(I,1),18X,5HBO(I)) SAVE 128
  780 FORMAT(8X,A2,5X,3E25.8)                                                SAVE 129
      WRITE(6,780)  (LLMT(I),BOP(I,2),BOP(I,1),BO(I),I=1,NLM)                SAVE 130
      RETURN                                                                 SAVE 131
      END                                                                    SAVE 132
```

```
C
      SUBROUTINE EQLBRM                                                      EQLM   1
C  ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES                 EQLM   2
C                                                                            EQLM   3
      DOUBLE PRECISION X,G,SUM                                               EQLM   4
C                                                                            EQLM   5
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR           EQLM   6
C     IBM 360 MACHINES ONLY                                                  EQLM   7
C                                                                            EQLM   8
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                      EQLM   9
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                                EQLM  10
C     DOUBLE PRECISION ENL,PROW,DLNT,AA                                      EQLM  11
C                                                                            EQLM  12
      LOGICAL HP,SP,TP,CONVG,IONS,SINGC,LOGV,ISING,IC,VOL,SHOCK,RITE         EQLM  13
C                                                                            EQLM  14
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)           EQLM  15
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),       EQLM  16
     2 VLM(13),TOTN(13)                                                      EQLM  17
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100),      EQLM  18
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)        EQLM  19
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),EQLM  20
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```
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),        EQLM  21
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),           EQLM  22
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),EQLM  23
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)        EQLM  24
      COMMON /DOUBLE/ G(20,21), X(20)                                     EQLM  25
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,     EQLM  26
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,  EQLM  27
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,  EQLM  28
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT             EQLM  29
C                                                                        EQLM  30
      EQUIVALENCE (NLM,L)                                                EQLM  31
C                                                                        EQLM  32
      DATA IE/1HE/,SMALNO/1.E-6/,SMNOL/-13.815511/,ITN/35/               EQLM  33
C                                                                        EQLM  34
      E = 2.718281828459                                                 EQLM  35
      SINGC = .FALSE.                                                    EQLM  36
      ENL = ENNL                                                         EQLM  37
      RITE = .FALSE.                                                     EQLM  38
      IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  RITE=.TRUE.                     EQLM  39
      SIZE = 18.420681                                                   EQLM  40
      ISING = .FALSE.                                                    EQLM  41
      LOGV = .FALSE.                                                     EQLM  42
      IF(.NOT.VOL) GO TO 6                                               EQLM  43
      RV = RR/101.325                                                    EQLM  44
      PP = RV*ENN*TT/VLM(NPT)                                            EQLM  45
    6 TLN = ALOG(TT)                                                     EQLM  46
      CONVG = .FALSE.                                                    EQLM  47
      ITNUMB = ITN                                                       EQLM  48
      JS1 = 1                                                            EQLM  49
      CALL CPHS                                                          EQLM  50
      TM = ALOG(PP/ENN)                                                  EQLM  51
C                                                                        EQLM  52
      IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                           EQLM  53
      L = L+1                                                            EQLM  54
      IQ1 = IQ1+1                                                        EQLM  55
      DO 499 J = 1,NS                                                    EQLM  56
      IF (A(L,J) .EQ.0.) GO TO 499                                       EQLM  57
      EN(J,NPT) = 1.E-8                                                  EQLM  58
      ENLN(J) = -SIZE                                                    EQLM  59
      IUSE(J) = 0                                                        EQLM  60
  499 CONTINUE                                                           EQLM  61
   33 IF(NPT.EQ.1.AND..NOT.SHOCK)   WRITE(6,244)(LLMT(I),I=1,L)          EQLM  62
  244 FORMAT (4HOPT ,14(5X,A4))                                          EQLM  63
C                                                                        EQLM  64
C     BEGIN ITERATION                                                    EQLM  65
C                                                                        EQLM  66
   42 IF (.NOT.CONVG)  GO TO 62                                          EQLM  67
      SUMN = ENN                                                         EQLM  68
      IF(JSOL.EQ.0)  GO TO 62                                            EQLM  69
      ENSOL = EN(JSOL,NPT)                                               EQLM  70
      EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)                           EQLM  71
      IUSE(JLIQ) = -IUSE(JLIQ)                                           EQLM  72
      IQ1 = IQ1-1                                                        EQLM  73
      DLVTP(NPT) = 0.                                                    EQLM  74
      CPR(NPT) = 0.                                                      EQLM  75
      GAMMAS(NPT) = 0.                                                   EQLM  76
      LOGV = .TRUE.                                                      EQLM  77
   62 CALL MATRIX                                                        EQLM  78
      NUMB = ITN-ITNUMB+1                                                EQLM  79
      IQ2 = IQ1 + 1                                                      EQLM  80
      IF(CONVG)  IMAT=IMAT-1                                             EQLM  81
      IF(.NOT.RITE)  GO TO 72                                            EQLM  82
      IF(.NOT.CONVG)  GO TO 88                                           EQLM  83
      IF(.NOT.LOGV)  WRITE(6,81)                                         EQLM  84
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   81 FORMAT(15HCT DERIV MATRIX)                                        EQLM  85
      IF(LOGV)  WRITE(6,82)                                             EQLM  86
   82 FORMAT(15HCP DERIV MATRIX)                                        EQLM  87
      GO TO 89                                                          EQLM  88
   88 WRITE(6,772) NUMB                                                 EQLM  89
  772 FORMAT (11HOITERATION  ,I3,6X,7HMATRIX //)                        EQLM  90
   89 DO 911 I=1,IMAT                                                   EQLM  91
  911 WRITE (6,73) (G(I,K),K=1,KMAT)                                    EQLM  92
   72 ITST = IMAT                                                       EQLM  93
      CALL GAUSS                                                        EQLM  94
      IF(ITST.NE.IMAT)  GO TO 774                                       EQLM  95
      IF(.NOT.RITE)  GO TO 773                                          EQLM  96
      WRITE (6,373)(LLMT(I),I=1,L)                                      EQLM  97
  373 FORMAT (7HOPI    ,9(A4,10X))                                      EQLM  98
      WRITE (6,73)(X(I),I=1,IMAT)                                       EQLM  99
   73 FORMAT (9E14.6)                                                   EQLM 100
  773 IF(.NOT.CONVG)  GO TO 85                                          EQLM 101
      IF(.NOT.LOGV)  GO TO 174                                          EQLM 102
      GO TO 171                                                         EQLM 103
C                                                                       EQLM 104
C     TEMPERATURE DERIVATIVES--CONVG=T, LOGV=F                          EQLM 105
C                                                                       EQLM 106
  174 DLVTP(NPT) = 1.-X(IQ1)                                            EQLM 107
      CPR(NPT) = G(IQ2,IQ2)                                             EQLM 108
      DO 176 J=1,IQ1                                                    EQLM 109
      CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)                                 EQLM 110
  176 CONTINUE                                                          EQLM 111
C                                                                       EQLM 112
C     PRESSURE DERIVATIVE--CONVG=T, LOGV=T                              EQLM 113
C                                                                       EQLM 114
      LOGV = .TRUE.                                                     EQLM 115
      GO TO 62                                                          EQLM 116
C                                                                       EQLM 117
C  SINGULAR MATRIX                                                      EQLM 118
C                                                                       EQLM 119
  774 IF(.NOT.CONVG)  GO TO 775                                         EQLM 120
      WRITE(6,172)                                                      EQLM 121
  172 FORMAT(28HODERIVATIVE MATRIX SINGULAR )                           EQLM 122
      GO TO 1171                                                        EQLM 123
  775 IF(.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 871       EQLM 124
      WRITE(6,874)                                                      EQLM 125
  874 FORMAT(96HOLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE  EQLM 126
     1BEEN INCLUDED ON AN INSERT CARD, RESTART )                        EQLM 127
      GO TO 873                                                         EQLM 128
  871 WRITE(6,74)                                                       EQLM 129
   74 FORMAT(16HOSINGULAR MATRIX)                                       EQLM 130
      IF(SINGC)  GO TO 873                                              EQLM 131
      DO 970 JJ = 1,NS                                                  EQLM 132
      IF(IUSE(JJ).NE.0)  GO TO 970                                      EQLM 133
      IF(EN(JJ,NPT).NE.0.)  GO TO 970                                   EQLM 134
      EN(JJ,NPT) = SMALNO                                               EQLM 135
      ENLN(JJ) = SMNOL                                                  EQLM 136
  970 CONTINUE                                                          EQLM 137
      IF(ISING)  GO TO 870                                              EQLM 138
      ISING = .TRUE.                                                    EQLM 139
      WRITE (6,776)                                                     EQLM 140
  776 FORMAT (8HORESTART)                                               EQLM 141
      GO TO 62                                                          EQLM 142
C                                                                       EQLM 143
C     TEST FOR SINGULARITY TO CONDENSED SPECIES.                        EQLM 144
C                                                                       EQLM 145
  870 NCCND = IQ1-NLM-1                                                 EQLM 146
      IF(NCCND.LT.2.OR.SIZEG.EQ.0.)  GO TO 873                          EQLM 148
      DO 872  J=1,NS                                                    EQLM 149
      IF(IUSE(J).LE.0)  GO TO 872                                       EQLM 150
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      IF(J.EQ.JDELG)  GO TO 872                                          EQLM 151
      DO 671  I=1,NLM                                                    EQLM 152
      IF(A(I,J).EQ.A(I,JDELG))  GO TO 671                                EQLM 153
      IF(A(I,J).EQ.0..OR.A(I,JDELG).EQ.0.)  GO TO 872                    EQLM 154
  671 CONTINUE                                                           EQLM 155
      SINGC = .TRUE.                                                     EQLM 156
      IQ1 = IQ1-1                                                        EQLM 157
      EN(J,NPT) = 0.                                                     EQLM 158
      IUSE(J) = -IUSE(J)                                                 EQLM 159
  872 CONTINUE                                                           EQLM 160
      IF(SINGC)  GO TO 40                                                EQLM 161
      GO TO 872                                                          EQLM 162
C                                                                        EQLM 163
C     OBTAIN CORRECTIONS TO THE ESTIMATES                                EQLM 164
C                                                                        EQLM 165
   85 ITNUMB= ITNUMB-1                                                   EQLM 166
      KK = L + 1                                                         EQLM 167
      IF(VOL)  X(IQ2)=X(IQ1)                                             EQLM 168
      IF(TP)  X(IQ2)=0.                                                  EQLM 169
      DLNT= X(IQ2)                                                       EQLM 170
      SUM = X(IQ1)                                                       EQLM 171
      IF(.NOT.VOL) GO TO 97                                              EQLM 172
      X(IQ1) = 0.                                                        EQLM 173
      SUM = -DLNT                                                        EQLM 174
   97 DO 101 J=1,NS                                                      EQLM 175
      IF (IUSE(J)) 101,98,100                                            EQLM 176
   98 DELN(J) = HO(J)*DLNT-HO(J)+S(J)-ENLN(J)-TM+SUM                     EQLM 177
      DO 99 K=1,L                                                        EQLM 178
      DELN(J)= DELN(J)+A(K,J)*X(K).                                      EQLM 179
   99 CONTINUE                                                           EQLM 180
      GO TO 101                                                          EQLM 181
  100 DELN(J) = X(KK)                                                    EQLM 182
      KK = KK + 1                                                        EQLM 183
  101 CONTINUE                                                           EQLM 184
C                                                                        EQLM 185
C     CALCULATE CONTROL FACTOR,AMBDA                                     EQLM 186
C                                                                        EQLM 187
      AMBDA= 1.                                                          EQLM 188
      AMBDA1= 1.                                                         EQLM 189
      SUM = X(IQ1)                                                       EQLM 190
      IF(SUM.LT.0.)  SUM=-SUM                                            EQLM 191
      IF(DLNT.GT.SUM)  SUM=DLNT                                          EQLM 192
      IF(-DLNT.GT.SUM)  SUM=-DLNT                                        EQLM 193
      DO 917 J=1,NS                                                      EQLM 194
      IF (IUSE(J).NE.0) GO TO 917                                        EQLM 195
      IF((EN(J,NPT).GT.0.).AND.DELN(J).GT.SUM) SUM = DELN(J)             EQLM 196
      IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GO TO 917                 EQLM 197
      SUM1 = (-9.212-ENLN(J)+ ENL)/(DELN(J)-X(IQ1))                      EQLM 198
      IF(SUM1.LT.0.)  SUM1=-SUM1                                         EQLM 199
      IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1                                  EQLM 200
  917 CONTINUE                                                           EQLM 201
      IF(SUM.GT.2.)AMBDA=2./SUM                                          EQLM 202
      IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1                                EQLM 203
      IF(.NOT.RITE)  GO TO 111                                           EQLM 204
C                                                                        EQLM 205
C     INTERMEDIATE OUTPUT                                                EQLM 206
C                                                                        EQLM 207
      WRITE(6,923) TT,ENN, ENL,PP,TM,AMBDA                               EQLM 208
  923 FORMAT (3HOT=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,   EQLM 209
     1 9H  LN P/N=E15.8,8H  AMBDA=E15.8 )                                EQLM 210
      IF(VOL)  WRITE(6,1924) VLM(NPT)                                    EQLM 211
 1924 FORMAT(8H VOLUME=,E15.8,4HCC/G)                                    EQLM 212
      WRITE (6,924)                                                      EQLM 213
  924 FORMAT(1HO,18X,2HNJ,12X,5HLN NJ,8X,9HDEL LN NJ,9X,6HHOJ/RT,9X,5HSOEQLM 214
     1J/R,10X,7H-GOJ/RT,8X,6H-GJ/RT  )                                   EQLM 215
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      DO 926 J=1,NS                                                    EQLM 216
      GNEG1 = S(J)-HO(J)                                               EQLM 217
      GNEG2 = GNEG1                                                    EQLM 218
      IF(IUSE(J).EQ.0)  GNEG2=GNEG2-ENLN(J)-TM                         EQLM 219
      WRITE (6,925) SUB(J,1),SUB(J,2),                                 EQLM 220
     1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),HO(J),S(J),GNEG1,GNEG2        EQLM 221
  925 FORMAT (1X,3A4,7E15.6)                                           EQLM 222
  926 CONTINUE                                                         EQLM 223
      WRITE (6,110)                                                    EQLM 224
  110 FORMAT(1HO)                                                      EQLM 225
C                                                                      EQLM 226
C     APPLY CORRECTIONS TO ESTIMATES                                   EQLM 227
C                                                                      EQLM 228
  111 SUM = 0.                                                         EQLM 229
      DO 113 J=1,NS                                                    EQLM 230
      IF (IUSE(J)) 113,112,114                                         EQLM 231
  112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)                                    EQLM 232
      EN(J,NPT) = 0.                                                   EQLM 233
      IF((ENLN(J)- ENL+SIZE).LE.0.)  GO TO 113                         EQLM 234
      EN(J,NPT) = E**ENLN(J)                                           EQLM 235
      SUM = SUM+EN(J,NPT)                                              EQLM 236
      GO TO 113                                                        EQLM 237
  114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)                          EQLM 238
  113 CONTINUE                                                         EQLM 239
      SUMN = SUM                                                       EQLM 240
      IF (TP) GO TO 115                                                EQLM 241
      TLN= TLN+AMBDA*DLNT                                              EQLM 242
      TT = EXP(TLN)                                                    EQLM 243
      JS1 = 1                                                          EQLM 244
      CALL CPHS                                                        EQLM 245
  115 IF(VOL) GO TO 2115                                               EQLM 246
      ENL = ENL+AMBDA*X(IQ1)                                           EQLM 247
      ENN = E**ENL                                                     EQLM 248
      GO TO 1115                                                       EQLM 249
 2115 ENN = SUMN                                                       EQLM 250
      ENL = ALOG(ENN)                                                  EQLM 251
      PP =  RV*TT*ENN/VLM(NPT)                                         EQLM 252
 1115 TM = ALOG(PP/ENN)                                                EQLM 253
      IF (LLMT(L).NE.IE) GO TO 116                                     EQLM 254
C                                                                      EQLM 255
C     CHECK ON REMOVING IONS                                           EQLM 256
C                                                                      EQLM 257
      DO 1116 J = 1,NS                                                 EQLM 258
      IF (A(L,J).EQ.0.) GO TO 1116                                     EQLM 259
      IF (EN(J,NPT).GT.0.) GO TO 116                                   EQLM 260
 1116 CONTINUE                                                         EQLM 261
      DO 1118  J=1,NS                                                  EQLM 262
      IF(A(L,J).NE.0.) IUSE(J) = -10000                                EQLM 263
 1118 CONTINUE                                                         EQLM 264
      L = L-1                                                          EQLM 265
      IQ1 = IQ1-1                                                      EQLM 266
      GO TO 43                                                         EQLM 267
C                                                                      EQLM 268
C     TEST FOR CONVERGENCE                                             EQLM 269
C                                                                      EQLM 270
  116 IF (ITNUMB.EQ.0) GO TO 14                                        EQLM 271
      IF (AMBDA.LT.1.) GO TO 43                                        EQLM 272
      SUM = (ENN-SUMN)/ENN                                             EQLM 273
      IF (SUM.LT.0.) SUM = -SUM                                        EQLM 274
      IF (SUM.GT.0.5E-5) GO TO 43                                      EQLM 275
      DO 130 J=1,NS                                                    EQLM 276
      IF (IUSE(J).LT.0) GO TO 130                                      EQLM 277
      AA= DELN(J)/SUMN                                                 EQLM 278
      IF(AA.LT.0.)  AA=-AA                                             EQLM 279
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      IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)                                EQLM 280
      IF(AA.GT.0.5E-5)  GO TO 43                                         EQLM 281
  130 CONTINUE                                                           EQLM 282
C                                                                        EQLM 283
C     CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS                EQLM 284
C                                                                        EQLM 285
      TOTN(NPT) = 0.                                                     EQLM 286
      SSUM(NPT) = 0.                                                     EQLM 287
      DO 183 J=1,NS                                                      EQLM 288
      IF(IUSE(J).LT.0)  GO TO 183                                        EQLM 289
      TOTN(NPT) = TOTN(NPT) + EN(J,NPT)                                  EQLM 290
      SS = S(J)                                                          EQLM 291
      IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-TM                                 EQLM 292
      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)                                 EQLM 293
  183 CONTINUE                                                           EQLM 294
      IF(.NOT.SP.OR.NPT.EQ.1)  GO TO 13                                  EQLM 295
      SS = SSUM(NPT) -SO                                                 EQLM 296
      IF(SS.LT.(-0.00005).OR.SS.GT.0.00005)  GO TO 43                    EQLM 297
      IF(RITE)  WRITE(6,1183)  SS                                        EQLM 298
 1183 FORMAT(12HODELTA S/R =,E15.8)                                      EQLM 299
C                                                                        EQLM 300
   13 CONVG= .TRUE.                                                      EQLM 301
      GO TO 160                                                          EQLM 302
   14 WRITE(6,973) ITN,NPT                                               EQLM 303
  973 FORMAT(1HL,I2,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMEEQLM 304
     1NTS FOR THE POINT       I5)                                        EQLM 305
      IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873       EQLM 306
      WRITE(6,874)                                                       EQLM 307
      GO TO 873                                                          EQLM 308
C                                                                        EQLM 309
C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.           EQLM 310
C                                                                        EQLM 311
  160 IF(NC.EQ.0) GO TO 143                                              EQLM 312
      DO 146  J=1,NS                                                     EQLM 313
      IF(EN(J,NPT).GE.0.)  GO TO 146                                     EQLM 314
      IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147                          EQLM 315
      JSOL = 0                                                           EQLM 316
      JLIQ = 0                                                           EQLM 317
  147 IQ1 = IQ1 - 1                                                      EQLM 318
      EN(J,NPT) = 0.                                                     EQLM 319
      GO TO 166                                                          EQLM 320
  146 CONTINUE                                                           EQLM 321
      SIZEG = 0.                                                         EQLM 322
      INC = 0                                                            EQLM 323
      DO 170 J = 1,NS                                                    EQLM 324
      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170                 EQLM 325
      INC = INC + 1                                                      EQLM 326
      IF(RITE)  WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),IUSEQLM 327
     1E(J),EN(J,NPT)                                                     EQLM 328
  144 FORMAT (1HO,3A4,2F10.3,3X,5HIUSE=,I4,E15.7)                        EQLM 329
      IF(EN(J,NPT).GT.0.)  GO TO 169                                     EQLM 330
      KG = 1                                                             EQLM 331
      IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154                                EQLM 332
      IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153                      EQLM 333
      KG = -1                                                            EQLM 334
  154 JKG = J + KG                                                       EQLM 335
      TMELT = TEMP(INC,1)                                                EQLM 336
      IMP = INC + KG                                                     EQLM 337
      IF(TMELT.EQ.TEMP(IMP,2)) GO TO 158                                 EQLM 338
      TMELT = TEMP(INC,2)                                                EQLM 339
      IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157                                EQLM 340
      WRITE (6,156)                                                      EQLM 341
  156 FORMAT (50HO3 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )    EQLM 342
      GO TO 873                                                          EQLM 343
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```
C  JTH SPECIES A SOLID (EN=0), (J+KG)TH SPECIES A LIQUID (EN IS +)
C
  157 IF(TT.GT.TMELT) GO TO 169
      IF (TP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP)  GO TO 1165
      IF (TT.LE.TMELT-150.) GO TO 1165
      JSOL = J
      JLIQ = JKG
      GO TO 159
C
C  JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)
C
  158 IF (TT.LT.TMELT) GO TO 169
      IF (TP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP)  GO TO 1165
      IF (TT.GE.TMELT+150.) GO TO 1165
      JSOL = JKG
      JLIQ = J
  159 TLN = ALOG (TMELT)
      TT = TMELT
      EN(JKG,NPT) = .5 * EN(JKG,NPT)
      EN(J,NPT) = EN(JKG,NPT)
      GO TO 165
C
C  WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
C
 1165 EN(J,NPT) = EN (JKG, NPT)
      IUSE(J) = -IUSE(J)
      IUSE (JKG) = -IUSE(JKG)
      EN(JKG,NPT)= 0.
      GO TO 40
  153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169
      IF (TT.GT.TEMP(INC,2)) GO TO 169
C
      SUM = 0.
      DO 167 I = 1,L
      SUM = SUM + A(I,J)*X(I)
  167 CONTINUE
      DELG = HC(J)-S(J)-SUM
      IF(RITE)  WRITE(6,168)DELG,SIZEG
  168 FORMAT (18H GO-SUM(AIJ*PII) =E15.7,10X,17HMAX NEG DELTA G =,E15.7)
      IF(DELG.GE.SIZEG .OR. DELG.GE.0.) GO TO 169
      SIZEG = DELG
      JDELG = J
  169 IF(INC.EQ.NC) GO TO 1160
  170 CONTINUE
 1160 IF (SIZEG.EQ.0.) GO TO 143
      J = JDELG
  165 IQ1 = IQ1 + 1
  166 IUSE(J) = - IUSE(J)
   40 CONVG = .FALSE.
      JS1 = 1
      CALL CPHS
  143 TN = NUME
      IF(.NOT.SHOCK)   WRITE(6,771)NPT,(X(IL),IL=1,L),TN
  771 FORMAT (I3,14F9.3)
      JS1 = 1
      IF(TP.AND.CONVG)  CALL CPHS
      ITNUMB = ITN
      GO TO 43
C
C     CALCULATE EQUILIBRIUM PROPERTIES
C
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C                                                                       EQLM 408
 1171 DLVPT(NPT) = -1.                                                  EQLM 409
      DLVTP(NPT) = 1.                                                   EQLM 410
      CPR(NPT) = CPSUM                                                  EQLM 411
      GO TO 199                                                         EQLM 412
  171 DLVPT(NPT) = -1. + X(IQ1)                                         EQLM 413
      IF(JLIQ.EQ.0)  GO TO 199                                          EQLM 414
      EN(JSOL,NPT) = ENSOL                                              EQLM 415
      IUSE(JLIQ) = -IUSE(JLIQ)                                          EQLM 416
      HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(HO(JLIQ)-HO(JSOL))            EQLM 417
      IQ1 = IQ1+1                                                       EQLM 418
      GAMMAS(NPT) = -1./DLVPT(NPT)                                      EQLM 419
      GO TO 186                                                         EQLM 420
  199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))       EQLM 421
  186 TTT(NPT) = TT                                                     EQLM 422
      ENNL = ENL                                                        EQLM 423
      PPP(NPT) = PP                                                     EQLM 424
      VLM(NPT) = RR*ENN*TT/(101.325*PP)                                 EQLM 425
      HSUM(NPT) = HSUM(NPT)*TT                                          EQLM 426
      WM(NPT) = 1./ENN                                                  EQLM 427
      IF(TRACE.EQ.0.)  GO TO 200                                        EQLM 428
      DO 1200  J=1,NS                                                   EQLM 429
      IF(IUSE(J).NE.0)  GO TO 1200                                      EQLM 430
      IF(ENLN(J).GT.-87.)  EN(J,NPT)=DEXP(ENLN(J))                      EQLM 431
 1200 CONTINUE                                                          EQLM 432
  200 IF(.NOT.RITE)  GO TO 863                                          EQLM 433
      WRITE(6,201)   NPT,PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NPT),    EQLM 434
     1 DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT),VLM(NPT)                       EQLM 435
  201 FORMAT (7HOPOINT=I3,3X,2HP=E13.6,3X,2HT=E13.6,3X,4HH/R=E13.6,3X,4HEQLM 436
     1S/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT=E13.6,3X,6HDLVEQLM 437
     2TP=E13.6,3X,9HGAMMA(S)=E13.6,3X,2HV=,E13.6)                       EQLM 438
  863 IF(TT.GE.TLOW.AND.TT.LE.THIGH.OR.SHOCK)  GO TO 1000               EQLM 439
      WRITE(6,306)  TT,NPT                                              EQLM 440
  306 FORMAT(17HOTHE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)EQLM 441
      IF(TT.GE.TLOW/1.5.AND.TT.LE.THIGH*1.25)  GO TO 1000               EQLM 442
      NPT = NPT+1                                                       EQLM 443
C                                                                       EQLM 444
C     ERROR, SET TT=0                                                   EQLM 445
C                                                                       EQLM 446
  873 TT=0.                                                             EQLM 447
      NPT = NPT-1                                                       EQLM 448
 1000 RETURN                                                            EQLM 449
      END                                                               EQLM 450
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C
      SUBROUTINE CPHS                                                   CPHS   1
C     CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES        CPHS   2
C                                                                       CPHS   3
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      CPHS   4
C     IBM 360 MACHINES ONLY                                             CPHS   5
C                                                                       CPHS   6
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           CPHS   7
C                                                                       CPHS   8
C                                                                       CPHS   9
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), CPHS  10
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   CPHS  11
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),CPHS  12
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      CPHS  13
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         CPHS  14
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),CPHS  15
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      CPHS  16
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM.   CPHS  17
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     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,  CPHS  18
     2 ICNS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,  CPHS  19
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT             CPHS  20
C                                                                        CPHS  21
      EQUIVALENCE (J,JS1)                                               CPHS  22
C                                                                        CPHS  23
      K = 1                                                             CPHS  24
      IF(TT.LE.TMID)   K = 2                                            CPHS  25
      KK = C                                                            CPHS  26
      CPSUM=0.                                                          CPHS  27
   90 IF(COEF(K,1,J).NE.0.)GO TO 97                                     CPHS  28
      IF (IUSE(J).LT.0) GO TO 100                                       CPHS  29
C                                                                        CPHS  30
C  IF COEFFICIENTS ARE ZERO, USE OTHER TEMPERATURE INTERVAL              CPHS  31
C                                                                        CPHS  32
      KK = K                                                            CPHS  33
      K = 1                                                             CPHS  34
      IF (KK.EQ.1)  K = 2                                               CPHS  35
   97 S(J) =  ((((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/  CPHS  36
     1 2.)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J)           CPHS  37
      HO(J) = ((((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/  CPHS  38
     1 3.) *TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J) + COEF(K,6,J)/TT        CPHS  39
      CPSUM= CPSUM+((((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF(K,3,J))*TT CPHS  40
     1 + COEF(K,2,J))*TT+ COEF(K,1,J))*EN(J,NPT)                        CPHS  41
      IF (KK.EQ.0) GO TO 100                                            CPHS  42
      K = KK                                                            CPHS  43
      KK = 0                                                            CPHS  44
  100 IF(J.EQ.NS) GO TO 200                                             CPHS  45
      J=J+1                                                             CPHS  46
      GO TO 90                                                          CPHS  47
  200 RETURN                                                            CPHS  48
      END                                                               CPHS  49
```

```
C                                                                        MATX   1
      SUBROUTINE MATRIX                                                  MATX   2
C                                                                        MATX   3
C                                                                        MATX   4
      DOUBLE PRECISION G,X                                               MATX   5
      LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR,VOL,UV,SV,TV,LOGV               MATX   6
C                                                                        MATX   7
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR       MATX   8
C     IBM 360 MACHINES ONLY                                              MATX   9
C                                                                        MATX  10
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                  MATX  11
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                            MATX  12
C     DOUBLE PRECISION H,F,SS,TERM1,TERM,SSS                             MATX  13
C                                                                        MATX  14
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),      MATX  15
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),   MATX  16
     2 VLM(13),TOTN(13)                                                 MATX  17
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100),  MATX  18
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   MATX  19
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2), MATX  20
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),       MATX  21
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),          MATX  22
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15), MATX  23
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      MATX  24
      COMMON /DOUBLE/ G(20,21), X(20)                                    MATX  25
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,    MATX  26
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```
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,  MATX  26
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JSI,VOL,IT,CALCH,NLS,LOGV,  MATX  27
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT             MATX  28
C                                                                        MATX  29
      EQUIVALENCE (NLM,L),(TP,TV),(SV,SP),(UV,HP)                       MATX  30
C                                                                        MATX  31
      IQ2 = IQ1 + 1                                                     MATX  32
      IQ3 = IQ2 + 1                                                     MATX  33
      KMAT = IQ3                                                        MATX  34
      IF(.NOT.CONVG.AND.TP) KMAT = IQ2                                  MATX  35
      IMAT = KMAT - 1                                                   MATX  36
C                                                                        MATX  37
C     CLEAR MATRIX STORAGES TO ZERO                                      MATX  38
C                                                                        MATX  39
      DO 211 I=1,IMAT                                                   MATX  40
      DO 211 K=1,KMAT                                                   MATX  41
      G(I,K)= 0.0D0                                                     MATX  42
  211 CONTINUE                                                          MATX  43
      SSS = 0.                                                          MATX  44
      HSUM(NPT) = 0.                                                    MATX  45
C                                                                        MATX  46
C     BEGIN SET UP OF ITERATION MATRIX                                   MATX  47
C                                                                        MATX  48
      KK = L                                                            MATX  49
      DO 65  J=1,NS                                                     MATX  50
      IF(IUSE(J).LT.0)  GO TO 65                                        MATX  51
      H=HO(J)*EN(J,NPT)                                                 MATX  52
      IF(IUSE(J).GT.0)  GO TO 70                                        MATX  53
      F = (HO(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                             MATX  54
      SS = H-F                                                          MATX  55
      TERM1 = H                                                         MATX  56
      IF (KMAT .EQ. IQ2) TERM1 = F                                      MATX  57
      DO 55 I = 1, L                                                    MATX  58
C                                                                        MATX  59
C     CALCULATE THE ELEMENTS  R(I,K)                                     MATX  60
C                                                                        MATX  61
      IF (A(I,J) .EQ. 0.) GO TO 55                                      MATX  62
      TERM= A(I,J)*EN(J,NPT)                                            MATX  63
      DO 15  K=I, L                                                     MATX  64
      G(I,K)= G(I,K) + A(K,J)*TERM                                      MATX  65
   15 CONTINUE                                                          MATX  66
C                                                                        MATX  67
      G(I,IQ1)=G(I,IQ1)+TERM                                            MATX  68
      G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                                    MATX  69
      IF (CONVG .OR.TP) GO TO 55                                        MATX  70
      G(I,IQ3)= G(I,IQ3)+A(I,J)*F                                       MATX  71
      IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS                           MATX  72
   55 CONTINUE                                                          MATX  73
      IF (KMAT .EQ. IQ2) GO TO 64                                       MATX  74
      IF(CONVG.OR.HP) GO TO 59                                          MATX  75
      G(IQ2,IQ1) = G(IQ2,IQ1) + SS                                      MATX  76
      G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS                                    MATX  77
      G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F                     MATX  78
      GO TO 62                                                          MATX  79
   59 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*H                                     MATX  80
      IF (CONVG) GO TO 64                                               MATX  81
      G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F                                     MATX  82
   62 G(IQ1,IQ3)=G(IQ1,IQ3)+F                                           MATX  83
   64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1                                       MATX  84
      GO TO 65                                                          MATX  85
C                                                                        MATX  86
C    CONDENSED SPECIES                                                  MATX  87
C                                                                        MATX  88
   70 KK = KK + 1                                                       MATX  89
      DO 75  I = I,L                                                    MATX  90
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      G(I,KK) = A(I,J)                                                  MATX  91
      G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)                          MATX  92
   75 CONTINUE                                                          MATX  93
      G(KK,IQ2) = HO(J)                                                 MATX  94
      G(KK,KMAT) = HO(J) - S(J)                                         MATX  95
      HSUM(NPT) = HSUM(NPT)+ H                                          MATX  96
      IF(.NOT.SP) GO TO 65                                              MATX  97
      SSS = SSS + S(J)*EN(J,NPT)                                        MATX  98
      G(IQ2,KK) = S(J)                                                  MATX  99
   65 CONTINUE                                                          MATX 100
      SSS = SSS + G(IQ2,IQ1)                                            MATX 101
      HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                                MATX 102
      G(IQ1,IQ1) = SUMN - ENN                                           MATX 103
C                                                                       MATX 104
C     REFLECT SYMMETRIC PORTIONS OF THE MATRIX                          MATX 105
C                                                                       MATX 106
      ISYM = IQ1                                                        MATX 107
      IF(HP.OR.CONVG)ISYM=IQ2                                           MATX 108
      DO 102 I=1,ISYM                                                   MATX 109
      DO 102 J=I,ISYM                                                   MATX 110
      G(J,I)=G(I,J)                                                     MATX 111
  102 CONTINUE                                                          MATX 112
C                                                                       MATX 113
C     COMPLETE THE RIGHT HAND SIDE                                      MATX 114
C                                                                       MATX 115
      IF(.NOT.CONVG)  GO TO 140                                         MATX 116
      IF(.NOT.LOGV)  GO TO 175                                          MATX 117
C                                                                       MATX 118
C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT                  MATX 119
C                                                                       MATX 120
      G(IQ1,IQ2) = ENN                                                  MATX 121
      IQ = IQ1 - 1                                                      MATX 122
      DO 135 I = 1,IQ                                                   MATX 123
      G(I,IQ2) = G(I,IQ1)                                               MATX 124
  135 CONTINUE                                                          MATX 125
      GO TO 175                                                         MATX 126
  140 DO 145 I=1,L                                                      MATX 127
      X(1)=BO(I)-G(I,IQ1)                                               MATX 128
      G(I,KMAT) = G(I,KMAT)+X(1)                                        MATX 129
  145 CONTINUE                                                          MATX 130
      G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                                MATX 131
C                                                                       MATX 132
C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN                        MATX 133
C                                                                       MATX 134
      IF (KMAT .EQ. IQ2) GO TO 185                                      MATX 135
      IF (SP)ENERGY = SO+ENN-SUMN - SSS                                 MATX 136
      IF(HP)ENERGY=HSUBO/TT - HSUM(NPT)                                 MATX 137
      G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                                     MATX 138
  175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                                      MATX 139
  185 IF(.NOT.VOL.OR.CONVG) GO TO 1000                                  MATX 140
C                                                                       MATX 141
C     CONSTANT VOLUME MATRIX                                            MATX 142
C                                                                       MATX 143
      IQ =IQ1-1                                                         MATX 144
      IF(KMAT.EQ.IQ2) GO TO 230                                         MATX 145
      DO 220 I=1,IQ                                                     MATX 146
      G(IQ1,I) = G(IQ2,I)-G(IQ1,I)                                      MATX 147
      G(I,IQ1) = G(I,IQ2)-G(I,IQ1)                                      MATX 148
      G(I,IQ2) = G(I,IQ3)                                               MATX 149
  220 CONTINUE                                                          MATX 150
      G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)                     MATX 151
      G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)                                MATX 152
      IF (UV) G(IQ1,IQ2) = G(IQ1,IQ2) + ENN                             MATX 153
      GO TO 260                                                         MATX 154
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  230 DO 240 I=1,IQ                                                    MATX 155
      G(I,IQ1) = G(I,IQ2)                                              MATX 156
  240 CONTINUE                                                         MATX 157
  260 KMAT = IMAT                                                      MATX 158
      IMAT = IMAT-1                                                    MATX 159
 1000 RETURN                                                           MATX 160
      END                                                              MATX 161
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C
      SUBROUTINE OUT1                                                  OUTP   1
C                                                                      OUTP   2
      DOUBLE PRECISION G,X                                             OUTP   3
C                                                                      OUTP   4
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR     OUTP   5
C     IBM 360 MACHINES ONLY                                            OUTP   6
C                                                                      OUTP   7
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                OUTP   8
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                          OUTP   9
C                                                                      OUTP  10
      LOGICAL EQL,FROZ,TP,HP,SP,HPSP,TPSP,MOLES,VOL,PUNCH,RKT          OUTP  11
C                                                                      OUTP  12
      DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5),FSB(3),FRHO(3)     OUTP  13
      DIMENSION DENSTY(13),ENTLPY(13),ENTRPY(13),SPHEAT(13)            OUTP  14
C                                                                      OUTP  15
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),    OUTP  16
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13), OUTP  17
     2 VLM(13),TOTN(13)                                                OUTP  18
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), OUTP  19
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)  OUTP  20
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),OUTP  21
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      OUTP  22
     2 HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),          OUTP  23
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),OUTP  24
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      OUTP  25
      COMMON /DOUBLE/ G(20,21), X(20)                                  OUTP  26
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,  OUTP  27
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, OUTP  28
     2 ICNS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, OUTP  29
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT          OUTP  30
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),       OUTP  31
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,      OUTP  32
     2 APPL,ARATIO,ELN                                                 OUTP  33
      COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,   OUTP  34
     1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,           OUTP  35
     2 FIRSTP,FIRSTV                                                   OUTP  36
      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),  OUTP  37
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2,        OUTP  38
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                        OUTP  39
      COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA                         OUTP  40
C                                                                      OUTP  41
      EQUIVALENCE (V,NV),(Z,HO),(IB,FB)                                OUTP  42
C                                                                      OUTP  43
C     HEAD=(1H ,2A4,5(A2,F8.5,3X),5X,F7.5,F13.3,4X,A1,F10.2,F9.4)      OUTP  44
C                                                                      OUTP  45
      DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX,    OUTP  46
     1 ,4HF7.5 ,4H,F13 ,4H.3,4 ,4HX,A1 ,4H,F10 ,4H.2,F ,4H9.4)/        OUTP  47
      DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,CX/1HO/,IZ/2H00/,      OUTP  48
     1 YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /,F75/4HF7.5/,                  OUTP  49
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     2 YX/3H,57,3H,44,3H,31,3H,18,2H,5 /,F73/4HF7.3/                    OUTP  50
      DATA FRHO/4HRHO,,4H G/C,1HC/                                      OUTP  51
C                                                                       OUTP  52
      IF(KASE.NE.0) WRITE (6,3) KASE                                    OUTP  53
    3 FORMAT (9H CASE NO. ,I8)                                          OUTP  54
      IF(.NOT.MOLES) WRITE(6,5)                                         OUTP  55
    5 FORMAT (77X,46HWT FRACTION   ENERGY   STATE   TEMP    DENSITY/    OUTP  56
     1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE)    CAL/MOL,10X,5HDEG K,OUTP  57
     2 4X,4HG/CC )                                                      OUTP  58
      IF(MOLES) WRITE(6,6)                                              OUTP  59
    6 FORMAT (79X,5HMOLES,7X,  33H ENERGY   STATE   TEMP    DENSITY/    OUTP  60
     1 10X,16HCHEMICAL FORMULA,66X,7HCAL/MOL,10X,13HDEG K    G/CC )     OUTP  61
      DO 15 N=1,NREAC                                                   OUTP  62
      IF(FOX(N).NE.OX)GO TO 10                                          OUTP  63
      HD1 = OXID                                                        OUTP  64
      HD2 = ANT                                                         OUTP  65
      GO TO 11                                                          OUTP  66
   10 HD1 = FUEL                                                        OUTP  67
      HD2 = FB                                                          OUTP  68
   11 DO 13 J=1,5                                                       OUTP  69
      IF(NAME(N,J).EQ.IZ.OR.NAME(N,J).EQ.IB)  GO TO 14                  OUTP  70
   13 CONTINUE                                                          OUTP  71
      J=6                                                               OUTP  72
   14 J=J-1                                                             OUTP  73
      HEAD(3)=YN(J)                                                     OUTP  74
      HEAD(7)=YX(J)                                                     OUTP  75
      HEAD(9) = F75                                                     OUTP  76
      IF(PECWT(N).GE.10.)  HEAD(9)=F73                                  OUTP  77
      WRITE(6,HEAD)  HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECWT(N),   OUTP  78
     1 ENTH(N), FAZ(N),RTEMP(N),DENS(N)                                 OUTP  79
   15 CONTINUE                                                          OUTP  80
      FPC = 100./(1.+OF)                                                OUTP  81
      WRITE(6,20)  OF,FPC,EQRAT,RHOP                                    OUTP  82
   20 FORMAT (1H0,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,        OUTP  83
     1  19HEQUIVALENCE RATIO= ,F7.4,4X,17HREACTANT DENSITY=,F8.4//)     OUTP  84
      AGV = 9.80665                                                     OUTP  85
C                                                                       OUTP  86
      RETURN                                                            OUTP  87
C                                                                       OUTP  88
      ENTRY OUT2                                                        OUTP  89
      FMT(4) = FMT(6)                                                   OUTP  90
C                                                                       OUTP  91
C   PRESSURE                                                            OUTP  92
C                                                                       OUTP  93
   50 IF(R.LT.10.)  GO TO 60                                            OUTP  94
      CALL EFMT(NPT,FP,PPP)                                             OUTP  95
      GO TO 64                                                          OUTP  96
   60 CALL VARFMT (PPP,NPT)                                             OUTP  97
      WRITE (6,FMT)  (FP(I),I=1,4),(PPP(J),J=1,NPT)                     OUTP  98
C                                                                       OUTP  99
C   TEMPERATURE                                                         OUTP 100
C                                                                       OUTP 101
   64 DO 65 I=1,NPT                                                     OUTP 102
      NV(I)= TTT(I)+.5                                                  OUTP 103
   65 CONTINUE                                                          OUTP 104
      FMT(4)= FMT13                                                     OUTP 105
      FMT(5)= FMTI9                                                     OUTP 106
      WRITE (6,FMT)  (FT(I),I=1,4),(NV(J),J=1,NPT)                      OUTP 107
C                                                                       OUTP 108
C   DENSITY                                                             OUTP 109
C                                                                       OUTP 110
      DO 70  I=1,NPT                                                    OUTP 111
      IF(VLM(I).NE.0.)  V(I)=1./VLM(I)                                  OUTP 112
      DENSTY(I) = V(I)                                                  OUTP 113
```

```
   70 CONTINUE                                                          OUTP 114
      CALL EFMT(NPT,FRHO,V)                                             OUTP 115
C                                                                       OUTP 116
C    ENTHALPY                                                           OUTP 117
C                                                                       OUTP 118
      DO 75 I=1,NPT                                                     OUTP 119
      V(I) = HSUM(I) * R                                                OUTP 120
      ENTLPY(I) = V(I)                                                  OUTP 121
   75 CONTINUE                                                          OUTP 122
      FMT(5)= FB                                                        OUTP 123
      IF(R.LT.10.) GO TO 76                                             OUTP 124
      CALL EFMT(NPT,FH,V)                                               OUTP 125
      FMT(7) = F1                                                       OUTP 126
      GO TO 77                                                          OUTP 127
   76 FMT(7) = F1                                                       OUTP 128
      WRITE (6,FMT)  (FH(I),I=1,4),(V(J),J=1,NPT)                       OUTP 129
C                                                                       OUTP 130
C    ENTROPY                                                            OUTP 131
C                                                                       OUTP 132
      FMT(7)=F4                                                         OUTP 133
   77 DO 78 I=1,NPT                                                     OUTP 134
      V(I) = SSUM(I) * R                                                OUTP 135
      ENTRPY(I) = V(I)                                                  OUTP 136
   78 CONTINUE                                                          OUTP 137
      WRITE (6,FMT)  (FS(I),I=1,4),(V(J),J=1,NPT)                       OUTP 138
      WRITE (6,80)                                                      OUTP 139
   80 FORMAT ( 1H )                                                     OUTP 140
C                                                                       OUTP 141
C    MOLECULAR WEIGHT                                                   OUTP 142
C                                                                       OUTP 143
      FMT(7)= F3                                                        OUTP 144
      WRITE (6,FMT)  (FM(I),I=1,4),(WM(J),J=1,NPT)                      OUTP 145
C                                                                       OUTP 146
C    (DLV/DLP)T                                                         OUTP 147
C                                                                       OUTP 148
      FMT(7)=F5                                                         OUTP 149
      IF(EQL) WRITE(6,FMT)  (FV(I),I=1,4),(DLVPT(J),J=1,NPT)            OUTP 150
C                                                                       OUTP 151
C    (DLV/DLT)P                                                         OUTP 152
C                                                                       OUTP 153
      FMT(7)= F4                                                        OUTP 154
      IF(EQL) WRITE(6,FMT)  (FD(I),I=1,4),(DLVTP(J),J=1,NPT)            OUTP 155
C                                                                       OUTP 156
C    HEAT CAPACITY                                                      OUTP 157
C                                                                       OUTP 158
      IF(R.GT.10.) FMT(7)=F1                                            OUTP 159
      DO 85  I=1,NPT                                                    OUTP 160
      V(I) = CPR(I) * R                                                 OUTP 161
      SPHEAT(I) = V(I)                                                  OUTP 162
   85 CONTINUE                                                          OUTP 163
      WRITE(6,FMT)  (FC(I),I=1,4),(V(J),J=1,NPT)                        OUTP 164
C                                                                       OUTP 165
C    GAMMA(S)                                                           OUTP 166
C                                                                       OUTP 167
      FMT(7) = F4                                                       OUTP 168
      WRITE(6,FMT)  (FG(I),I=1,4),(GAMMAS(J),J=1,NPT)                   OUTP 169
C                                                                       OUTP 170
C    SONIC VELOCITY                                                     OUTP 171
C                                                                       OUTP 172
      FMT(7)= F1                                                        OUTP 173
      DO 95 I = 1,NPT                                                   OUTP 174
      SONVEL(I) = (RR*GAMMAS(I)*TTT(I)/WM(I))**.5                       OUTP 175
   95 CONTINUE                                                          OUTP 176
      WRITE(6,FMT)  (FL(I),I=1,4),(SONVEL(J),J=1,NPT)                   OUTP 177
```

```
C                                                                       OUTP 178
C     PUNCHED CARDS                                                     OUTP 179
C                                                                       OUTP 180
      IF(.NOT.PUNCH) GO TO 4                                            OUTP 181
      DO 1 I=1,NPT                                                      OUTP 182
      IF(RKT.AND.ISV.EQ.0.AND.MAXNP.GT.0.AND.(I.EQ.1.OR.I.EQ.2)) GO TO 1OUTP 183
      PUNCH 2, TTT(I),PPP(I),DENSTY(I),ENTLPY(I),ENTRPY(I),WM(I),       OUTP 184
     1 DLVPT(I),CLVTP(I),V(I),GAMMAS(I),SONVEL(I),FPC                   OUTP 185
    2 FORMAT (F8.2,2(3X,E10.5),F11.2,F11.4,F11.5/2F11.6,F11.5,F11.6,    OUTP 186
     1 F10.2,2X,F8.4)                                                   OUTP 187
    1 CONTINUE                                                          OUTP 188
C                                                                       OUTP 189
    4 RETURN                                                            OUTP 190
C                                                                       OUTP 191
      ENTRY OUT3                                                        OUTP 192
C                                                                       OUTP 193
      TRA = 5.E-6                                                       OUTP 194
      IF(TRACE.NE.0.)  TRA= TRACE                                       OUTP 195
      IF(.NOT.EQL)  GO TO 331                                           OUTP 196
C                                                                       OUTP 197
C   MOLE FRACTIONS - EQUILIBRIUM                                        OUTP 198
C                                                                       OUTP 199
      WRITE (6,80)                                                      OUTP 200
      FMT(7)= F5                                                        OUTP 201
      WRITE(6,310)                                                      OUTP 202
  310 FORMAT(15HOMOLE FRACTIONS //)                                     OUTP 203
      DO 330 K=1,NS                                                     OUTP 204
      DO 315 I=1,NPT                                                    OUTP 205
      V(I) = EN(K,I)/TOTN(I)                                            OUTP 206
  315 CONTINUE                                                          OUTP 207
      DO 316 I=1,NPT                                                    OUTP 208
      IF(TRACE.EQ.0.)  GO TO 317                                        OUTP 209
      IF(V(I).GE.TRACE)  GO TO 325                                      OUTP 210
  317 IF(V(I).GE.(5.E-6))  GO TO 320                                    OUTP 211
  316 CONTINUE                                                          OUTP 212
      GO TO 330                                                         OUTP 213
  320 WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT)        OUTP 214
      GO TO 330                                                         OUTP 215
  325 FSB(1) = SUB(K,1)                                                 OUTP 216
      FSB(2) = SUB(K,2)                                                 OUTP 217
      FSB(3) = SUB(K,3)                                                 OUTP 218
      CALL EFMT(NPT,FSB,V)                                              OUTP 219
  330 CONTINUE                                                          OUTP 220
  331 WRITE(6,335) TRA                                                  OUTP 221
  335 FORMAT(83HOADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLOUTP 222
     1B FRACTIONS WERE LESS THAN ,E12.5,28H FOR ALL ASSIGNED CONDITIONS/OUTP 223
     2/)                                                                OUTP 224
      LINE= 0                                                           OUTP 225
      NN = 1                                                            OUTP 226
      IF(EQL)  NN=NPT                                                   OUTP 227
      DO 350 K=1,NS                                                     OUTP 228
      DO 340  I=1,NN                                                    OUTP 229
      IF ((EN(K,I)/TOTN(I)).GE.TRA)  GO TO 343                          OUTP 230
  340 CONTINUE                                                          OUTP 231
      LINE= LINE+1                                                      OUTP 232
      Z(LINE,1)= SUB(K,1)                                               OUTP 233
      Z(LINE,2)= SUB(K,2)                                               OUTP 234
      Z(LINE,3)= SUB(K,3)                                               OUTP 235
  343 IF ((LINE.NE.10) .AND. K.NE.NS) GO TO 350                         OUTP 236
      IF (LINE.EQ.0) GO TO 1000                                         OUTP 237
      WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)                  OUTP 238
  345 FORMAT (10(1X,3A4))                                               OUTP 239
      LINE= 0                                                           OUTP 240
  350 CONTINUE                                                          OUTP 241
      IF(.NOT.MOLES) WRITE(6,360)                                       OUTP 242
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  360 FORMAT(78HONOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIOUTP 243
     2DANT IN TOTAL OXIDANTS    )                                        OUTP 244
 1000 RETURN                                                            OUTP 245
      END                                                               OUTP 246
```

```
C
      SUBROUTINE VARFMT(V,NPT)                                          VRFT   1
C                                                                       VRFT   2
      DIMENSION V(13)                                                   VRFT   3
C                                                                       VRFT   4
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),    VRFT   5
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,         VRFT   6
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                         VRFT   7
C                                                                       VRFT   8
      DO 45 I=1,NPT                                                     VRFT   9
      K= 2*I+3                                                          VRFT  10
      FMT(K) = F4                                                       VRFT  11
      IF (V(I).GE.10.) FMT(K) = F3                                      VRFT  12
      IF (V(I).GE.100.) FMT(K) = F2                                     VRFT  13
      IF (V(I).GE.10000.)FMT(K) = F1                                    VRFT  14
      IF (V(I).GE.1000000.) FMT(K) = F0                                 VRFT  15
   45 CONTINUE                                                          VRFT  16
      RETURN                                                            VRFT  17
      END                                                               VRFT  18
```

```
C
      SUBROUTINE EFMT(NPT,AA,V)                                         EFMT   1
C                                                                       EFMT   2
      DIMENSION AA(3), V(13), W(13), NE(13), FRMT(7)                    EFMT   3
C                                                                       EFMT   4
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),    EFMT   5
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,         EFMT   6
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                         EFMT   7
C                                                                       EFMT   8
      DATA FRMT/3H(1H,4H,3A4,4H,11X,4H,13(,4HF7.4,4H,I2),1H)/,F63/4HF6.3EFMT   9
     1/,FI3/4H,I3)/,F74/4HF7.4/,FI2/4H,I2)/,F11X/4H,11X/,F2X/3H,2X/     EFMT  10
C                                                                       EFMT  11
      FRMT(5) = F74                                                     EFMT  12
      FRMT(6) = FI2                                                     EFMT  13
      J1 = 1                                                            EFMT  14
      FRMT(3) = F2X                                                     EFMT  15
      IF(FMT(4).NE.FMT9X)  GO TO 130                                    EFMT  16
      J1 = 2                                                            EFMT  17
      FRMT(3) = F11X                                                    EFMT  18
  130 DO 145  I=J1,NPT                                                  EFMT  19
      IF(V(I).NE.0.) GO TO 140                                          EFMT  20
      W(I) = 0.                                                         EFMT  21
      NE(I) = 0.                                                        EFMT  22
      GO TO 145                                                         EFMT  23
  140 EE = ALOG10(ABS(V(I)))                                            EFMT  24
      NE(I) = EE                                                        EFMT  25
      FE = NE(I)                                                        EFMT  26
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```
      IF(EE.LE.0..AND.FE.NE.EE)  NE(I)=NE(I)-1                          EFMT  27
      IF(IABS(NE(I)).LT.10)  GO TO 144                                  EFMT  28
      FRMT(5) = F63                                                     EFMT  29
      FRMT(6) = FI3                                                     EFMT  30
  144 W(I) = V(I)/10.**NE(I)                                            EFMT  31
  145 CONTINUE                                                          EFMT  32
      WRITE(6,FRMT)  (AA(I),I=1,3),(W(J), NE(J),J=J1,NPT)               EFMT  33
 1000 RETURN                                                            EFMT  34
      END                                                               EFMT  35
```

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C
      SUBROUTINE THERMP (*)                                             THRP   1
C                                                                       THRP   2
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      THRP   3
C     IBM 360 MACHINES ONLY                                             THRP   4
C                                                                       THRP   5
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                 THRP   6
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           THRP   7
C                                                                       THRP   8
      LOGICAL HP,SP,TP,UV,SV,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,  THRP   9
     1 CALCH                                                            THRP  10
C                                                                       THRP  11
      DIMENSION VL(26)                                                  THRP  12
C                                                                       THRP  13
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     THRP  14
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  THRP  15
     2 VLM(13),TOTN(13)                                                 THRP  16
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), THRP  17
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   THRP  18
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),THRP  19
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      THRP  20
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         THRP  21
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),THRP  22
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      THRP  23
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   THRP  24
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, THRP  25
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JSI,VOL,IT,CALCH,NLS,LOGV, THRP  26
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            THRP  27
      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),   THRP  28
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,         THRP  29
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FC                         THRP  30
C                                                                       THRP  31
      EQUIVALENCE (K,ISV ),(VL,P),(UV,HP),(TP,TV),(SP,SV)               THRP  32
C                                                                       THRP  33
      DATA FUU/4HU, C/                                                  THRP  34
C                                                                       THRP  35
      IF(T(1).EQ.0.)  T(1) = 3800.                                      THRP  36
C                                                                       THRP  37
      IOF = 0                                                           THRP  38
   95 IOF = IOF+1                                                       THRP  39
      OF = OXF(IOF)                                                     THRP  40
      CALL NEWCF                                                        THRP  41
      IF(TT.EQ.0..AND.CALCH)  RETURN 1                                  THRP  42
C                                                                       THRP  43
C     SET ASSIGNED P OR VOLUME                                          THRP  44
C                                                                       THRP  45
      IP = 0                                                            THRP  46
  903 IP =IP + 1                                                        THRP  47
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      PP = P(IP)                                                        THRP  48
      VLM(NPT) = VL(IP)                                                 THRP  49
C                                                                       THRP  50
C     SET ASSIGNED T                                                    THRP  51
C                                                                       THRP  52
      IT = 0                                                            THRP  53
  902 IT = IT + 1                                                       THRP  54
      TT = T(IT)                                                        THRP  55
      CALL EQLBRM                                                       THRP  56
      IF(TT.NE.0.)  GO TO 800                                           THRP  57
      IF(NPT.EQ.0)  GO TO 1000                                          THRP  58
  800 K = 0                                                             THRP  59
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860                  THRP  60
      K = NPT                                                           THRP  61
      IF(NPT.NE.13)  GO TO 870                                          THRP  62
  860 IF(.NOT.HP)  WRITE(6,5)                                           THRP  63
    5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNEDTHRP  64
     1)                                                                 THRP  65
      IF(HP)  WRITE(6,6)                                                THRP  66
    6 FORMAT(1H1,36X,59HTHERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES THRP  67
     1AT ASSIGNED  )                                                    THRP  68
      IF(.NOT.VOL)  GO TO 861                                           THRP  69
      IF(UV)  WRITE(6,10)                                               THRP  70
   10 FORMAT(1HO,62X,7H VOLUME /)                                       THRP  71
      IF(TV)  WRITE(6,11)                                               THRP  72
   11 FORMAT(1HO,54X,22HTEMPERATURE AND VOLUME/)                        THRP  73
      IF(SV)  WRITE(6,12)                                               THRP  74
   12 FORMAT(1HO,56X,18HENTROPY AND VOLUME/)                            THRP  75
      GO TO 862                                                         THRP  76
  861 IF(HP)  WRITE(6,20)                                               THRP  77
   20 FORMAT(1HO,62X,10H PRESSURES  /)                                  THRP  78
      IF(TP)  WRITE(6,21)                                               THRP  79
   21 FORMAT(1HO,53X,24HTEMPERATURE AND PRESSURE/)                      THRP  80
      IF(SP)  WRITE(6,22)                                               THRP  81
   22 FORMAT(1HO,55X,20HENTROPY AND PRESSURE/)                          THRP  82
  862 CALL OUT1                                                         THRP  83
      WRITE (6,863)                                                     THRP  84
  863 FORMAT (25HOTHERMODYNAMIC PROPERTIES//)                           THRP  85
      IF(.NOT.VOL)  GO TO 864                                           THRP  86
      FMT(4) = FMT(6)                                                   THRP  87
      IF(.NOT.UV) GO TO 864                                             THRP  88
      DO 63 I=1,NPT                                                     THRP  89
      FMT(2*I+3) = F2                                                   THRP  90
      V(I) = HSUBO*R                                                    THRP  91
   63 CONTINUE                                                          THRP  92
      WRITE(6,FMT) FUU,FH(2),FB,FB,(V(I),I=1,NPT)                       THRP  93
  864 CALL OUT2                                                         THRP  94
      CALL OUT3                                                         THRP  95
C                                                                       THRP  96
      RETURN                                                            THRP  97
C                                                                       THRP  98
      ENTRY THERM1                                                      THRP  99
C                                                                       THRP 100
  865 IF(K.EQ.0 .AND. IOF.EQ.NOF) GO TO 1000                            THRP 101
      IF(IDEBUG.GT.13)  IDEBUG=IDEBUG-13                                THRP 102
      WRITE(6,868)                                                      THRP 103
  868 FORMAT(1H1)                                                       THRP 104
      IF(NT.EQ.1.AND.NP.EQ.1)  GO TO 95                                 THRP 105
      NPT = 0                                                           THRP 106
  870 NPT = NPT + 1                                                     THRP 107
      IF(.NOT.TP.AND.TT.NE.0.)  T(1)=TT                                 THRP 108
      IF(IP.EQ.1.AND.IT.EQ.1)  ISV=-ISV                                 THRP 109
      IF(NT.EQ.1)  GO TO 871                                            THRP 110
      IF(IT.EQ.NT.OR.TT.EQ.0.)  ISV=0                                   THRP 111
  871 CALL SAVE                                                         THRP 112
      IF(IT.LT.NT) GO TO 902                                            THRP 113
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      IF(IP.LT.NP) GO TO 903                                            THRP 114
      GO TO 95                                                          THRP 115
 1000 RETURN 1                                                          THRP 116
      END                                                               THRP 117
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C
      SUBROUTINE ROCKET (*)                                             ROCK   1
C                                                                       ROCK   2
C     ROCKET PERFORMANCE                                                ROCK   3
C                                                                       ROCK   4
      DOUBLE PRECISION USQ,ASQ                                          ROCK   5
C                                                                       ROCK   6
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR       ROCK   7
C     IBM 360 MACHINES ONLY                                             ROCK   8
C                                                                       ROCK   9
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                 ROCK  10
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           ROCK  11
C                                                                       ROCK  12
      LOGICAL HP,SP,TP,THI,FROZ,EQL,AREA,SEQL,CALCH                     ROCK  13
C                                                                       ROCK  14
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     ROCK  15
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  ROCK  16
     2 VLM(13),TCTN(13)                                                 ROCK  17
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), ROCK  18
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   ROCK  19
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BC(10),BOP(10,2),ROCK  20
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      ROCK  21
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         ROCK  22
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),ROCK  23
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      ROCK  24
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   ROCK  25
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, ROCK  26
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, ROCK  27
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            ROCK  28
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        ROCK  29
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       ROCK  30
     2 APPL,ARATIO,ELN                                                  ROCK  31
                                                                        ROCK  32
C                                                                       ROCK  33
C                                                                       ROCK  34
      NAMELIST/RKTINP/EQL,FROZ,SUBAR,SUPAR,PCP,NFZ                      ROCK  35
C                                                                       ROCK  36
      ITM = 1                                                           ROCK  37
      NFZ = 1                                                           ROCK  38
      APP(1) = 1.                                                       ROCK  39
      DO 300 I=1,26                                                     ROCK  40
      PCP(I)= 0.                                                        ROCK  41
      SUBAR(I) = 0.                                                     ROCK  42
  300 CONTINUE                                                          ROCK  43
      EQL = .TRUE.                                                      ROCK  44
      FROZ = .TRUE.                                                     ROCK  45
      READ (5,RKTINP)                                                   ROCK  46
      NPP = 0                                                           ROCK  47
      DO 305 I=1,22                                                     ROCK  48
      IF(PCP(I).EQ.0.) GO TO 306                                        ROCK  49
      NPP = I                                                           ROCK  50
  305 CONTINUE                                                          ROCK  51
  306 NPP = NPP+2                                                       ROCK  52
  311 NSUB = 0                                                          ROCK  53
      NSUP = 0
```

```
      DO 320  I=1,13                                                    ROCK  54
      IF(SUBAR(I).NE.0.) NSUB=NSUB+1                                    ROCK  55
      IF(SUPAR(I).NE.0.) NSUP=NSUP+1                                    ROCK  56
  320 CONTINUE                                                          ROCK  57
      WRITE (6,RKTINP)                                                  ROCK  58
      SEQL = EQL                                                        ROCK  59
      IOF = 0                                                           ROCK  60
      TT = 3800.                                                        ROCK  61
C                                                                       ROCK  62
C     LOOP FOR EACH O/F                                                 ROCK  63
C                                                                       ROCK  64
  321 IT = 1                                                            ROCK  65
      IOF = IOF + 1                                                     ROCK  66
      OF = OXF(IOF)                                                     ROCK  67
      CALL NEWOF                                                        ROCK  68
      IF(CALCH.AND.TT.EQ.0.)  RETURN 1                                  ROCK  69
      IF(T(1).EQ.0.)  GO TO 322                                         ROCK  70
      TT = T(1)                                                         ROCK  71
C                                                                       ROCK  72
C     LOOP FOR CHAMBER PRESSURES                                        ROCK  73
C                                                                       ROCK  74
  322 IP = 0                                                            ROCK  75
  998 IP =IP + 1                                                        ROCK  76
      ITNUM = 0                                                         ROCK  77
      AREA = .FALSE.                                                    ROCK  78
      IF(T(1).EQ.0.)  HP=.TRUE.                                         ROCK  79
      IF(T(1).NE.0.)  TP=.TRUE.                                         ROCK  80
      SP = .FALSE.                                                      ROCK  81
      EQL = .TRUE.                                                      ROCK  82
      ISUB = 1                                                          ROCK  83
      ISUP = 1                                                          ROCK  84
      PP = P(IP)                                                        ROCK  85
      IPP = 1                                                           ROCK  86
      ITROT = 3                                                         ROCK  87
      ISUPSV = 1                                                        ROCK  88
C                                                                       ROCK  89
C     LOOP FOR PRESSURE RATIOS                                          ROCK  90
C                                                                       ROCK  91
  331 IF(EQL)  GO TO 332                                                ROCK  92
      CALL FROZEN                                                       ROCK  93
      GO TO 1332                                                        ROCK  94
  332 CALL EQLBRM                                                       ROCK  95
      IF(NPT.NE.NFZ) GO TO 1332                                         ROCK  96
      CPRF = CPSUM                                                      ROCK  97
      IF(NFZ.NE.2) EQL = SEQL                                           ROCK  98
C                                                                       ROCK  99
C     TT = 0 IF NO CONVERGENCE                                          ROCK 100
C                                                                       ROCK 101
 1332 IF(TT.NE.0.)  GO TO 333                                           ROCK 102
      IF(NPT.LT.1)  GO TO 1000                                          ROCK 103
      GO TO 900                                                         ROCK 104
  333 IF(IPP.GT.1) GO TO 195                                            ROCK 105
C                                                                       ROCK 106
C     COMBUSTION CHAMBER                                                ROCK 107
C                                                                       ROCK 108
      TP = .FALSE.                                                      ROCK 109
      HP = .FALSE.                                                      ROCK 110
      SP = .TRUE.                                                       ROCK 111
      SO = SSUM(1)                                                      ROCK 112
  334 TMELT=0.                                                          ROCK 113
      ITROT= 3                                                          ROCK 114
      THI = .FALSE.                                                     ROCK 115
      APP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))           ROCK 116
      PP = PPP(1)/APP(2)                                                ROCK 117
      TT = 2.*TT/(GAMMAS(1)+1.)                                         ROCK 118
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      ISV = 1                                                          ROCK 119
      GO TO 870                                                        ROCK 120
  195 USQ = 2.*(HSUM(1)-HSUM(NPT)) * RR                                ROCK 121
      IF (IPP.GT.2) GO TO 900                                          ROCK 122
C                                                                      ROCK 123
C     THROAT                                                           ROCK 124
C                                                                      ROCK 125
  190 IF(.NOT.THI)  GO TO 191                                          ROCK 126
      GAMMAS(2) = 0.                                                   ROCK 127
      GO TO 899                                                        ROCK 128
  191 ASQ = GAMMAS(2)*TT*ENN*RR                                        ROCK 129
      IF(EQL)  WRITE(6,194) APP(2),TT                                  ROCK 130
  194 FORMAT (7H PC/PT= , F9.6, 6H    T = , F9.2)                      ROCK 131
      IF(IDEBUG.EQ.1.OR.IDEBUG.EQ.2)  WRITE(6,923)USQ,ASQ              ROCK 132
  923 FORMAT(5HOUSQ=,E15.8,5X,4HASQ=,E15.8)                            ROCK 133
      DH = (USQ-ASQ)/ASQ                                               ROCK 134
      IF(DH.LT.0.)  DH=-DH                                             ROCK 135
      IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GO TO 899                        ROCK 136
      IF(JSOL.NE.0) GO TO 925                                          ROCK 137
      IF(TMELT.EQ.0.) GO TO 192                                        ROCK 138
      DLT = ALOG(TMELT/TT)                                             ROCK 139
      DD = DLT*CPR(2)/(ENN*DLVTP(2))                                   ROCK 140
      PP = EXP(DD)                                                     ROCK 141
      APP(2) = P(IP)/PP                                                ROCK 142
      THI = .TRUE.                                                     ROCK 143
      GO TO 331                                                        ROCK 144
  925 TMELT = TT                                                       ROCK 145
  192 APP(2)= APP(2)/(1.+(USQ-ASQ)/(ENN*TT*RR*(GAMMAS(2)+1.)))        ROCK 146
  193 PP = P(IP)/APP(2)                                                ROCK 147
      ITROT = ITROT-1                                                  ROCK 148
      GO TO 331                                                        ROCK 149
  899 AWT =ENN*TT/(PP*USQ**.5)                                         ROCK 150
      PCPLT = ALOG(APP(2))                                             ROCK 151
      IF(NFZ.EQ.2) EQL = SEQL                                          ROCK 152
  900 ISV =0                                                           ROCK 153
      AEAT(NPT) = ENN*TTT(NPT)/(PP*USQ**.5*AWT)                        ROCK 154
      IF(TT.EQ.0.)  GO TO 860                                          ROCK 155
      IF(AREA)  GO TO 800                                              ROCK 156
      IF(IPP.LT.NPP)  GO TO 859                                        ROCK 157
  788 IF(NSUB.LE.0.AND.NSUP.EQ.0) GO TO 860                            ROCK 158
      AREA = .TRUE.                                                    ROCK 159
C                                                                      ROCK 160
C     PCP ESTIMATES FOR AREA RATIOS                                    ROCK 161
C                                                                      ROCK 162
  800 IF(ITNUM.NE.0)  GO TO 810                                        ROCK 163
      DLNP = 1.                                                        ROCK 164
      ITNUM = 1                                                        ROCK 165
      ARATIO = SUBAR(ISUB)                                             ROCK 166
      IF(NSUB.LE.0)  ARATIO=SUPAR(ISUP)                                ROCK 167
      IF(EQL.OR.NFZ.LT.3) GO TO 798                                    ROCK 168
      IF(ARATIO.GT.AEAT(NFZ)) GO TO 798                                ROCK 169
      WRITE(6,884)                                                     ROCK 170
      GO TO 834                                                        ROCK 171
  798 ELN = ALOG(ARATIO)                                               ROCK 172
      IF(NSUB.LE.0)  GO TO 799                                         ROCK 173
      APPL = PCPLT/(SUBAR(ISUB)+(10.587*ELN**2+9.454)*ELN)             ROCK 174
      IF(ARATIO.LT.1.09)  APPL=.9*APPL                                 ROCK 175
      IF(ARATIO.GT.10.) APPL=APPL/ARATIO                               ROCK 176
      GO TO 859                                                        ROCK 177
  799 IF(NFZ.EQ.IPP) ISUPSV = ISUP                                     ROCK 178
      IF(SUPAR(ISUP).LT.2.)  GO TO 805                                 ROCK 179
      IF(ISUP.GT.1.AND.SUPAR(ISUP-1).GE.2.)  GO TO 802                 ROCK 180
      APPL = GAMMAS(2)+ELN*1.4                                         ROCK 181
      GO TO 859                                                        ROCK 182
  805 APPL = SQRT(ELN*(1.535+3.294*ELN))+PCPLT                         ROCK 183
      GO TO 859                                                        ROCK 184
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C                                                                       ROCK 185
C     TEST FOR CONVERGENCE ON AREA RATIO.                               ROCK 186
C                                                                       ROCK 187
  810 CHECK = .00004                                                    ROCK 188
      IF(IDEBUG.LE.0.OR.NPT.LT.IDEBUG)  GO TO 809                       ROCK 189
      WRITE(6,1811)ITNUM,ARATIO,AEAT(NPT),APP(NPT),DLNP                 ROCK 190
 1811 FORMAT (6HOITER=,I2,5X,15HASSIGNED AE/AT=,F15.8,5X,6HAE/AT=,F15.8,ROCK 191
     15X,5HPC/P=,F15.8,5X,13HDELTA LN PCP=,F15.8)                       ROCK 192
  809 IF(ABS(AEAT(NPT)-  ARATIO). /ARATIO  .LE.CHECK)    GO TO 830      ROCK 193
      DELTAE = (AEAT(NPT)-ARATIO)/ARATIO                                ROCK 194
      IF(ABS(DLNP).LT..00004)  GO TO 830                                ROCK 195
      AEATL= ALOG(AEAT(NPT))                                            ROCK 196
  811 ITNUM = ITNUM+1                                                   ROCK 197
      IF(ITNUM.GT.10)  GO TO 840                                        ROCK 198
C                                                                       ROCK 199
C     IMPROVED PCP ESTIMATES                                            ROCK 200
C                                                                       ROCK 201
      ASQ = GAMMAS(NPT)*ENN*RR*TT                                       ROCK 202
      DLNPE = GAMMAS(NPT)*USQ/(USQ-ASQ)                                 ROCK 203
  802 DLNP = DLNPE*ELN-DLNPE*AEATL                                      ROCK 204
      APPL = APPL+DLNP                                                  ROCK 205
      IF(ITNUM.EQ.1)  GO TO 859                                         ROCK 206
      APP(NPT) = EXP(APPL)                                              ROCK 207
      PP = P(IP)/APP(NPT)                                               ROCK 208
      GO TO 331                                                         ROCK 209
C                                                                       ROCK 210
  830 ITNUM = 0                                                         ROCK 211
      AEAT(NPT) = ARATIO                                                ROCK 212
      IF(NSUB.LE.0)  GO TO 834                                          ROCK 213
      ISUB = ISUB+1                                                     ROCK 214
      IF(ISUB.LE.NSUB)  GO TO 800                                       ROCK 215
      ISUB = 1                                                          ROCK 216
      NSUB = -NSUB                                                      ROCK 217
      IF(ISUP.LE.NSUP)  GO TO 800                                       ROCK 218
      GO TO 835                                                         ROCK 219
  834 ISUP = ISUP+1                                                     ROCK 220
      ITNUM = 0                                                         ROCK 221
      IF(ISUP.LE.NSUP)  GO TO 800                                       ROCK 222
      ISUP = ISUPSV                                                     ROCK 223
  835 AREA = .FALSE.                                                    ROCK 224
      GO TO 860                                                         ROCK 225
  840 WRITE(6,841) ARATIO                                               ROCK 226
  841 FORMAT(34HODID NOT CONVERGE FOR AREA RATIO =,F10.5)               ROCK 227
      GO TO 830                                                         ROCK 228
C                                                                       ROCK 229
C     TEST FOR OUTPUT -- END OF PCP,SUBAR,AND SUPAR SCHEDULES OR NPT=13.ROCK 230
C                                                                       ROCK 231
  859 ISV = NPT                                                         ROCK 232
      IF(NPT.NE.13)  GO TO 870                                          ROCK 233
  860 IF(EQL) GO TO 861                                                 ROCK 234
      IF(NFZ.GT.1) GO TO 861                                            ROCK 235
      CPR(NFZ) = CPRF                                                   ROCK 236
      GAMMAS(NFZ) = CPRF/(CPRF-1./WM(NFZ))                              ROCK 237
C                                                                       ROCK 238
  861 CALL RKTOUT                                                       ROCK 239
C                                                                       ROCK 240
      IF (TT.EQ.0.) ISV = 0                                             ROCK 241
C                                                                       ROCK 242
      RETURN                                                            ROCK 243
C                                                                       ROCK 244
      ENTRY ROCKT1                                                      ROCK 245
C                                                                       ROCK 246
      DLNP = 1.                                                         ROCK 247
      IF(.NOT.EQL.AND.TT.EQ.0.)  WRITE(6,862)                           ROCK 248
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  862 FORMAT(105HOCALCULATIONS WERE STOPPED BECAUSE NEXT POINT IS MORE TROCK 249
     1HAN 50 DEG BELOW TEMP RANGE OF A CONDENSED SPECIES)                ROCK 250
      IF (ISV.EQ.0) GO TO 990                                            ROCK 251
      IF(IDEBUG.GT.13) IDEBUG = IDEBUG-13                                ROCK 252
      IF(EQL)  WRITE(6,865)                                              ROCK 253
  865 FORMAT(1H1)                                                        ROCK 254
      NPT = 2                                                            ROCK 255
C                                                                        ROCK 256
C     SET INDICES AND ESTIMATES FOR NEXT POINT.                          ROCK 257
C                                                                        ROCK 258
  870 NPT = NPT + 1                                                      ROCK 259
      IF(.NOT.EQL.AND.(ISV.NE.1.OR.SEQL)) GO TO 880                      ROCK 260
      IF(ISV.EQ.1)  ISV = -1                                             ROCK 261
      CALL SAVE                                                          ROCK 262
  880 IPP = IPP+1                                                        ROCK 263
      IF(NPT.EQ.2)  GO TO 331                                            ROCK 264
      IF(AREA) GO TO 885                                                 ROCK 265
      APP(NPT) = PCP(IPP-2)                                              ROCK 266
      IF(EQL) GO TO 886                                                  ROCK 267
      IF(APP(NPT).GE.APP(NFZ)) GO TO 886                                 ROCK 268
      WRITE(6,884)                                                       ROCK 269
  884 FORMAT(//,1X,114HSUPERSONIC PRESSURE RATIOS MUST BE IN ASCENDING ORROCK 270
     1DER    POINTS OUT OF ORDER WERE OMITTED FROM FROZEN CALCULATIONS)ROCK 271
      GO TO 880                                                          ROCK 272
  885 APP(NPT) = EXP(APPL)                                               ROCK 273
  886 PP = P(IP)/APP(NPT)                                                ROCK 274
      GO TO 331                                                          ROCK 275
C                                                                        ROCK 276
C     END OF PCP, SUBAR, AND SUPAR SCHEDULES.                            ROCK 277
C                                                                        ROCK 278
  990 IF(NSUB.LT.0)  NSUB=-NSUB                                          ROCK 279
      IF (.NOT.FROZ.OR..NOT.EQL)  GO TO 997                              ROCK 280
C                                                                        ROCK 281
C     SET UP FOR FROZEN.                                                 ROCK 282
C                                                                        ROCK 283
      EQL = .FALSE.                                                      ROCK 284
      CALL SAVE                                                          ROCK 285
      TT = TTT(NFZ)                                                      ROCK 286
      IPP = NFZ                                                          ROCK 287
      IF(NFZ.EQ.NPT) GO TO 860                                           ROCK 288
      NPT = NFZ                                                          ROCK 289
      ENN = 1./WM(NFZ)                                                   ROCK 290
      IF(NFZ.EQ.1) GO TO 334                                             ROCK 291
      NSUB = -NSUB                                                       ROCK 292
      IF(APP(NFZ).GE.APP(2)) GO TO 994                                   ROCK 293
      WRITE(6,993)                                                       ROCK 294
  993 FORMAT (//,28X,77HFREEZING IS NOT ALLOWED AT A SUBSONIC POINT, FROROCK 295
     1ZEN CALCULATIONS WERE OMITTED)                                     ROCK 296
      GO TO 997                                                          ROCK 297
  994 IF(NFZ.LT.NPP) GO TO 870                                           ROCK 298
      GO TO 788                                                          ROCK 299
  997 NPT = 1                                                            ROCK 300
C                                                                        ROCK 301
C     ARE THERE MORE ASSIGNED,                                           ROCK 302
C      1) CHAMBER PRESSURES(IP = NP)                                     ROCK 303
C      2) CHAMBER TEMPERATURES(IT = NT)                                  ROCK 304
C      3) O/F VALUES(IOF = NOF)                                          ROCK 305
C                                                                        ROCK 306
      IF(IP.EQ.NP.AND.IT.EQ.NT.AND.IOF.EQ.NOF)  GO TO 1000               ROCK 307
      WRITE(6,865)                                                       ROCK 308
      IF(SEQL) CALL SAVE                                                 ROCK 309
      TT = TTT(1)                                                        ROCK 310
      IF(IP.LT.NP) GO TO 998                                             ROCK 311
      IF(IT.GE.NT)  GO TO 999                                            ROCK 312
      IT = IT+1                                                          ROCK 313
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      TT = T(IT)                                                        ROCK 314
      GO TO 322                                                         ROCK 315
  999 IF (IOF.GE.NOF)  GO TO 1000                                       ROCK 316
      GO TO 321                                                         ROCK 317
 1000 RETURN 1                                                          ROCK 318
      END                                                               ROCK 319
```

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C
      SUBROUTINE RKTOUT                                                 ROUT   1
C                                                                       ROUT   2
C  ROCKET PERFORMANCE PARAMETERS                                        ROUT   3
C                                                                       ROUT   4
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      ROUT   5
C     IBM 360 MACHINES ONLY                                             ROUT   6
C                                                                       ROUT   7
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                 ROUT   8
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           ROUT   9
C                                                                       ROUT  10
      LOGICAL EQL,FROZ ,TP,HP,SP,SHOCK,AREA                             ROUT  11
C                                                                       ROUT  12
      DIMENSION NV(13),Z(10,4)                                          ROUT  13
C                                                                       ROUT  14
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     ROUT  15
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  ROUT  16
     2 VLM(13),TOTN(13)                                                 ROUT  17
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), ROUT  18
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   ROUT  19
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),ROUT  20
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      ROUT  21
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         ROUT  22
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FCX(15),DENS(15),ROUT  23
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      ROUT  24
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   ROUT  25
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, ROUT  26
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, ROUT  27
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            ROUT  28
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        ROUT  29
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       ROUT  30
     2 APPL,ARATIO,ELN                                                  ROUT  31
      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),   ROUT  32
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,         ROUT  33
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                         ROUT  34
C                                                                       ROUT  35
      EQUIVALENCE (V,NV),(Z,HO)                                         ROUT  36
C                                                                       ROUT  37
      DATA EXIT/4HEXIT/                                                 ROUT  38
C                                                                       ROUT  39
      IF(.NOT.EQL)  GO TO 636                                           ROUT  40
      WRITE(6,37)                                                       ROUT  41
   37 FORMAT(1H1/24X,84HTHEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRROUT  42
     1IUM COMPOSITION DURING EXPANSION                                  ROUT  43
      GO TO 39                                                          ROUT  44
  636 WRITE(6,38)                                                       ROUT  45
   38 FORMAT(1H1,26X,78HTHEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN CROUT  46
     1OMPOSITION DURING EXPANSION                                       ROUT  47
      IF(NFZ.GT.1)  WRITE(6,637)NFZ                                     ROUT  48
  637 FORMAT(58X,11HAFTER POINT,I2)                                     ROUT  49
   39 IF(TTT(1).EQ.T(IT)) WRITE(6,737)                                  ROUT  50
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  737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE                          ROUT  51
      TEM = PPP(1)*14.696006                                             ROUT  52
      WRITE (6,40) TEM                                                   ROUT  53
   40 FORMAT(5HOPC = ,F8.1,5H PSIA)                                      ROUT  54
      CALL OUT1                                                          ROUT  55
      NEX = NPT - 2                                                      ROUT  56
      DO 862 I = 1,NEX                                                   ROUT  57
  862 V(I) = EXIT                                                        ROUT  58
      WRITE(6,48) (V(I),I=1,NEX)                                         ROUT  59
   48 FORMAT(1HO,16X,16HCHAMBER    THROAT   ,11(5X,A4))                  ROUT  60
C                                                                        ROUT  61
C   PRESSURE RATIOS                                                      ROUT  62
C                                                                        ROUT  63
      FMT(4) = FMT(6)                                                    ROUT  64
      CALL VARFMT (APP,NPT)                                              ROUT  65
      WRITE (6,FMT) FR1,FB,FB,FB,(APP(J),J=1,NPT)                        ROUT  66
      CALL OUT2                                                          ROUT  67
C                                                                        ROUT  68
      AGV = 9.80665                                                      ROUT  69
      DO 202 K=2,NPT                                                     ROUT  70
      SPIM(K) = (2.*RR*(HSUM(1)-HSUM(K)))**.5/AGV                        ROUT  71
C                                                                        ROUT  72
C   AW (A/W) IN UNITS OF SEC/ATM                                         ROUT  73
C                                                                        ROUT  74
      AW = RR*TTT(K)/(PPP(K)*WM(K)*SPIM(K)*AGV**2)                       ROUT  75
      IF(K.NE.2)GO TO 200                                                ROUT  76
      CSTR = 32.174*PPP(1)*AW                                            ROUT  77
      AEAT(2) = 1.                                                       ROUT  78
  200 VACI(K)=SPIM(K)+PPP(K)*AW                                          ROUT  79
      IF (SONVEL(K).NE.0.) VMOC(K)=SPIM(K)*AGV/SONVEL(K)                 ROUT  80
      NV(K)= CSTR + .5                                                   ROUT  81
  202 CONTINUE                                                           ROUT  82
C                                                                        ROUT  83
C   MACH NUMBER                                                          ROUT  84
C                                                                        ROUT  85
      VMOC(1)=0.                                                         ROUT  86
      IF(GAMMAS(2).EQ.0.) VMOC(2)=0.                                     ROUT  87
      FMT(7) = F3                                                        ROUT  88
      WRITE(6,FMT)  (FN(I),I=1,4),(VMOC(J),J=1,NPT)                      ROUT  89
      WRITE (6,208)                                                      ROUT  90
  208 FORMAT (1H )                                                       ROUT  91
C                                                                        ROUT  92
C   AREA RATIO                                                           ROUT  93
C                                                                        ROUT  94
      FMT(4) = FMT9X                                                     ROUT  95
      CALL VARFMT (AEAT,NPT)                                             ROUT  96
      FMT(5) = FB                                                        ROUT  97
      WRITE(6,FMT)  FA1,FA2,FB,FB,(AEAT(J),J=2,NPT)                      ROUT  98
C                                                                        ROUT  99
C   C*                                                                   ROUT 100
C                                                                        ROUT 101
      FMT(5) = FMT13                                                     ROUT 102
      FMT(6) = FMTI9                                                     ROUT 103
      FMT(7) = FB                                                        ROUT 104
      WRITE(6,FMT)  (FR(I),I=1,4),(NV(J),J=2,NPT)                        ROUT 105
C                                                                        ROUT 106
C   CF - THRUST COEFICIENT                                               ROUT 107
C                                                                        ROUT 108
      FMT(6) = FMT(8)                                                    ROUT 109
      FMT(7) = F3                                                        ROUT 110
      DO 212  I=2,NPT                                                    ROUT 111
  212 V(I)=32.174*SPIM(I)/CSTR                                           ROUT 112
      WRITE(6,FMT)  FC1,FB,FB,FB,(V(J),J=2,NPT)                          ROUT 113
C                                                                        ROUT 114
C   VACUUM IMPULSE                                                       ROUT 115
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C                                                                       ROUT 116
      FMT(5) = FMT13                                                    ROUT 117
      FMT(7) = F1                                                       ROUT 118
      WRITE(6,FMT)  (FA(I),I=1,4),(VACI(J),J=2,NPT)                     ROUT 119
C                                                                       ROUT 120
C   SPECIFIC IMPULSE                                                    ROUT 121
C                                                                       ROUT 122
      WRITE(6,FMT)  (FI(I),I=1,4),(SPIM(J),J=2,NPT)                     ROUT 123
      WRITE (6,208)                                                     ROUT 124
      FMT(4) = F8                                                       ROUT 125
      FMT(5) = FMT13                                                    ROUT 126
      FMT(7) = F5                                                       ROUT 127
      IF(EQL)  GO TO 312                                                ROUT 128
      WRITE(6,310)                                                      ROUT 129
  310 FORMAT(15HOMOLE FRACTIONS //)                                     ROUT 130
C                                                                       ROUT 131
C   MOLE FRACTIONS - FROZEN                                             ROUT 132
C                                                                       ROUT 133
      TRA = 5.E-6                                                       ROUT 134
      IF(TRACE.NE.0.)  TRA=TRACE                                        ROUT 135
      LINE = 0                                                          ROUT 136
      DO 430 K =1,NS                                                    ROUT 137
      V(LINE+1) = EN(K,NFZ)/TOTN(NFZ)                                   ROUT 138
      IF(V(LINE+1).LT.TRA)  GO TO 424                                   ROUT 139
      LINE = LINE+1                                                     ROUT 140
      Z(LINE,1) = SUB(K,1)                                              ROUT 141
      Z(LINE,2) = SUB(K,2)                                              ROUT 142
      Z(LINE,3) = SUB(K,3)                                              ROUT 143
      Z(LINE,4) = V(LINE)                                               ROUT 144
  424 IF (LINE.NE.4.AND.K.NE.NS)  GO TO 430                             ROUT 145
      IF (LINE.EQ.0)  GO TO 312                                         ROUT 146
      WRITE (6,426) (Z(LN,1),Z(LN,2),Z(LN,3),Z(LN,4),LN=1,LINE)         ROUT 147
  426 FORMAT (1H ,4(3A4,F9.5,7X))                                       ROUT 148
      LINE = 0                                                          ROUT 149
  430 CONTINUE                                                          ROUT 150
  312 CALL OUT2                                                         ROUT 151
 1000 RETURN                                                            ROUT 152
      END                                                               ROUT 153
```

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C                                                                       FROZ   1
      SUBROUTINE FROZEN                                                 FROZ   2
C                                                                       FROZ   3
C     (FROZEN COMPOSITION EXPANSION ONLY)                               FROZ   4
C                                                                       FROZ   5
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      FROZ   6
C     IBM 360 MACHINES ONLY                                             FROZ   7
C                                                                       FROZ   8
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                 FROZ   9
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           FROZ  10
C     DOUBLE PRECISION SUMS,SUMH,SS                                     FROZ  11
C                                                                       FROZ  12
      LOGICAL EQL,FROZ,CONVG,SP,HP,VOL                                  FROZ  13
C                                                                       FROZ  14
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     FROZ  15
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  FROZ  16
     2 VLM(13),TOTN(13)                                                 FROZ  17
      COMMON /SPECES/COEF(2,7  00),S(100),HO(100),DELN(100),DUMMY(100). FROZ  18
     1 EN(100,13),ENLN(100),A( 0,100),SUB(100,3),IUSE(100),TEMP(50,2)   FROZ  19
```

```
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),FROZ  19
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),        FROZ  20
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),           FROZ  21
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),FROZ  22
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)        FROZ  23
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,     FROZ  24
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,  FROZ  25
     2 ICNS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,  FROZ  26
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT              FROZ  27
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),          FROZ  28
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,         FROZ  29
     2 APPL,ARATIO,ELN                                                    FROZ  30
      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),     FROZ  31
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,           FROZ  32
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                           FROZ  33
C                                                                         FROZ  34
      CONVG = .FALSE.                                                     FROZ  35
      TLN = ALOG(TT)                                                      FROZ  36
      DO 51  ITER=1,8                                                     FROZ  37
      SUMS = 0.                                                           FROZ  38
      SUMH = 0.                                                           FROZ  39
      JS1 = ITM                                                           FROZ  40
      NNN = NPT                                                           FROZ  41
      NPT = NFZ                                                           FROZ  42
      CALL CPHS                                                           FROZ  43
      CC = CPSUM                                                          FROZ  44
   55 NPT = NNN                                                           FROZ  45
      DO 60 J=ITM,NS                                                      FROZ  46
      IF (EN(J,NFZ).EQ.0.) GO TO 60                                       FROZ  47
      PMN = PP*WM(NFZ)*EN(J,NFZ)                                          FROZ  48
      SS = S(J)                                                           FROZ  49
      IF(IUSE(J).EQ.0)  SS=SS-ALOG(PMN)                                   FROZ  50
      SUMS = SUMS+SS*EN(J,NFZ)                                            FROZ  51
      IF (CONVG)  SUMH=SUMH+HO(J)*EN(J,NFZ)                               FROZ  52
   60 CONTINUE                                                            FROZ  53
      IF (CONVG) GO TO 81                                                 FROZ  54
      DLNT=(SUMS-SO)/CC                                                   FROZ  55
      TLN=TLN-DLNT                                                        FROZ  56
      IF(DLNT.LT.0.) DLNT=-DLNT                                           FROZ  57
      IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.                                    FROZ  58
      TT = EXP(TLN)                                                       FROZ  59
   51 CONTINUE                                                            FROZ  60
      WRITE(6,70)                                                         FROZ  61
   70 FORMAT(40HOFROZEN DID NOT CONVERGE IN 8 ITERATIONS)                 FROZ  62
      GO TO 903                                                           FROZ  63
   81 TTT(NPT)= TT                                                        FROZ  64
      SSUM(NPT)= SUMS                                                     FROZ  65
      HSUM(NPT)= TT*SUMH                                                  FROZ  66
      GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(NFZ))                               FROZ  67
      VLM(NPT) = RR*TT/(WM(NFZ)*101.325*PP)                               FROZ  68
      WM(NPT) = WM(NFZ)                                                   FROZ  69
C                                                                         FROZ  70
      DLVPT(NPT) = -1.                                                    FROZ  71
      DLVTP(NPT) = 1.                                                     FROZ  72
      TOTN(NPT) = TOTN(NFZ)                                               FROZ  73
      PPP(NPT) = PP                                                       FROZ  74
      CPR(NPT) = CPSUM                                                    FROZ  75
      IF (TT.LT.(TLOW-150.))GO TO 903                                     FROZ  76
      IF(NC.EQ.0) GO TO 1000                                              FROZ  77
      INC =0                                                              FROZ  78
      DO 901  I=ITM,NS                                                    FROZ  79
      IF(IUSE(I).EQ.0.OR.IUSE(I).EQ.-10000) GO TO 901                     FROZ  80
      INC = INC+1                                                         FROZ  81
      IF (EN(I,NFZ).EQ.0.) GO TO 901                                      FROZ  82
      IF(TT.LT.(TEMP(INC,1)-50.).OR.TT.GT.(TEMP(INC,2)+50.))GO TO 903     FROZ  83
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  901 CONTINUE                                                          FROZ  84
      GO TO 1000                                                        FROZ  85
  903 TT=0.                                                             FROZ  86
      NPT= NPT-1                                                        FROZ  87
 1000 RETURN                                                            FROZ  88
      END                                                               FROZ  89
```

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C
      SUBROUTINE SHCK (*)                                               SHCK   1
C                                                                       SHCK   2
      DOUBLE PRECISION G,X,GG                                           SHCK   3
C                                                                       SHCK   4
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR      SHCK   5
C     IBM 360 MACHINES ONLY                                             SHCK   6
C                                                                       SHCK   7
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                 SHCK   8
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                           SHCK   9
C                                                                       SHCK  10
      REAL MACH1,M1,MACH2,M2,M12,M5,M25,MACHO ,MU12RT,M2M1              SHCK  11
      LOGICAL INCDEQ,INCDFZ,REFLEQ,REFLFZ,TP,FROZ,EQL,SECL,MOLES,       SHCK  12
     1 SHOCK,SREFL,REFL,CALCH                                           SHCK  13
C                                                                       SHCK  14
      DIMENSION NUM(15,5),FV2(4),FUV(4),W(10)                           SHCK  15
      DIMENSION M2M1(13),T2T1(13),U1U2(13),RRHO(13),SG(78),U5(13)       SHCK  16
      DIMENSION U1(13),MACH1(13),UTWO(13),Z(10,3),U2STAR(13)            SHCK  17
C                                                                       SHCK  18
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     SHCK  19
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  SHCK  20
     2 VLM(13),TOTN(13)                                                 SHCK  21
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), SHCK  22
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   SHCK  23
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),SHCK  24
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      SHCK  25
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         SHCK  26
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),SHCK  27
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      SHCK  28
      COMMON /DOUBLE/ G(20,21), X(20)                                   SHCK  29
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   SHCK  30
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, SHCK  31
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JSI,VOL,IT,CALCH,NLS,LOGV, SHCK  32
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            SHCK  33
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        SHCK  34
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       SHCK  35
     2 APPL,ARATIO,ELN                                                  SHCK  36
      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),   SHCK  37
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2,         SHCK  38
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                         SHCK  39
C                                                                       SHCK  40
      EQUIVALENCE(M2M1,AEAT),(T2T1,SPIM),(U1U2,VACI,U2STAR),(U1,SUBAR)  SHCK  41
      EQUIVALENCE (SG,G(4,3)), (APP ,RRHO),(Z,HO),(ANUM,NUM),(U5, UTWO) SHCK  42
     1 ,(GG,X(4)),(MACH1,SUPAR),(M1,DATA(20)),(CPR1,DATA(21))           SHCK  43
      EQUIVALENCE (REFL,ISUP),(NSK,ISUB)                                SHCK  44
C                                                                       SHCK  45
      NAMELIST /SHKINP/U1,MACH1,GAMMA1,INCDEQ,REFLEQ,INCDFZ,REFLFZ,A1   SHCK  46
      DATA ONE/1H1/,                  FPP/4HP2/P/, FTT/4HT2/T/          SHCK  47
     2     FU1/3HU1/ /, FMM/4HM2/M/, FRA/4HRHO2/, FRB/4H/RHO/           SHCK  48
     3     FMA/4HMACH/, FMB/4H NO./, IZERO/2H00/,FU2/3HU2,/              SHCK  49
      DATA TWO/1H2/,   FP5/4HP5/P/, FT5/4HT5/T/                         SHCK  50
     2   FU5/3HU5,/,  FM5/4HM5/M/,FR5/4HRHO5/                          SHCK  51
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```
      DATA FV2/4HV2(U,4H1-U2,4H)M/S,2HEC/                               SHCK  52
     1   ,  FUV/4HU5+V, 4H2,M/,3HSEC,1H /                               SHCK  53
C                                                                       SHCK  54
      NFZ = 1                                                           SHCK  55
      CALCH = .FALSE.                                                   SHCK  56
      IF(TRACE.EQ.0.)  TRACE=5.E-9                                      SHCK  57
      IOF = 0                                                           SHCK  58
      TP=.TRUE.                                                         SHCK  59
      CPR1 = 0.                                                         SHCK  60
      DO 10 I=1,13                                                      SHCK  61
      MACH1(I)=0.                                                       SHCK  62
      U1(I)=0.                                                          SHCK  63
   10 CONTINUE                                                          SHCK  64
      GAMMA1 = 0.                                                       SHCK  65
      INCDEQ = .TRUE.                                                   SHCK  66
      INCDFZ = .TRUE.                                                   SHCK  67
      REFLEQ = .FALSE.                                                  SHCK  68
      REFLFZ = .FALSE.                                                  SHCK  69
      DO 18 N = 1,NREAC                                                 SHCK  70
      NAME(N,5) = IZERO                                                 SHCK  71
   18 CONTINUE                                                          SHCK  72
      SREFL = .FALSE.                                                   SHCK  73
      READ (5,SHKINP)                                                   SHCK  74
      WRITE(6,SHKINP)                                                   SHCK  75
      IF(REFLEQ.OR.REFLFZ)  SREFL=.TRUE.                                SHCK  76
      SEQL = INCDEQ                                                     SHCK  77
      IF(T(1).EQ.0.)  T(1)=RTEMP(1)                                     SHCK  78
      DO 20 I = 1,13                                                    SHCK  79
      IF (MACH1(I).EQ.0.0.AND.U1(I).EQ.0.0) GO TO 21                    SHCK  80
      NSK = I                                                           SHCK  81
   20 CONTINUE                                                          SHCK  82
   21 IOF = IOF+1                                                       SHCK  83
      OF = OXF(IOF)                                                     SHCK  84
      CALL NEWOF                                                        SHCK  85
C                                                                       SHCK  86
      INCDEQ = SEQL                                                     SHCK  87
   17 REFL = .FALSE.                                                    SHCK  88
      IT2 = 2                                                           SHCK  89
      IT1 = 1                                                           SHCK  90
      PP = P(1)                                                         SHCK  91
      TT = T(1)                                                         SHCK  92
C                                                                       SHCK  93
C  FROZEN                                                               SHCK  94
C                                                                       SHCK  95
  117 DO 118 N = 1,NSK                                                  SHCK  96
      DLVTP(N) = 1.                                                     SHCK  97
      DLVPT(N) = -1.                                                    SHCK  98
      DO 118 J = 1,NS                                                   SHCK  99
      EN(J,N) = 0.0                                                     SHCK 100
  118 CONTINUE                                                          SHCK 101
C                                                                       SHCK 102
   19 DO 35  NPT=1,NSK                                                  SHCK 103
      PPP(NPT) = P(NPT)                                                 SHCK 104
      TTT(NPT) = T(NPT)                                                 SHCK 105
      IF(NPT.EQ.1)  GO TO 14                                            SHCK 106
      IF(PPP(NPT).EQ.0.)  PPP(NPT)=PPP(NPT-1)                           SHCK 107
      IF(TTT(NPT).EQ.0.)  TTT(NPT)=TTT(NPT-1)                           SHCK 108
      SSUM(NPT) = SSUM(NPT-1)                                           SHCK 109
      HSUM(NPT) = HSUM(NPT-1)                                           SHCK 110
      IF(TTT(NPT).EQ.TT.AND.PPP(NPT).EQ.PP)  GO TO 15                   SHCK 111
   14 PP = PPP(NPT)                                                     SHCK 112
      TT = TTT(NPT)                                                     SHCK 113
      IF(TT.GE.TLOW/1.5)  GO TO 814                                     SHCK 114
      WRITE(6,1152)                                                     SHCK 115
      GO TO 1000                                                        SHCK 116
```

```
  814 CALL HCALC                                                        SHCK 117
      HSUM(NPT) = HSUBO                                                 SHCK 118
   15 IF(CPR1.NE.0.)  GAMMA1=CPR1/(CPR1-1./M1)                          SHCK 119
      A1 = (RR*GAMMA1*TT/M1)**.5                                        SHCK 120
   31 IF(U1(NPT).EQ.0.)  U1(NPT)=A1*MACH1(NPT)                          SHCK 121
      IF (MACH1(NPT).EQ.0.) MACH1(NPT) = U1(NPT)/A1                     SHCK 122
      WM(NPT) = M1                                                      SHCK 123
      CPR(NPT) = CPR1                                                   SHCK 124
      GAMMAS(NPT) = GAMMA1                                              SHCK 125
      VLM(NPT) = RR*TT/(M1*101.325*PP)                                  SHCK 126
   35 CONTINUE                                                          SHCK 127
C                                                                       SHCK 128
C  OUTPUT--1ST CONDITION                                                SHCK 129
C                                                                       SHCK 130
      WRITE (6,861)                                                     SHCK 131
  861 FORMAT(1H1,48X,30HSHOCK WAVE PARAMETERS ASSUMING    )             SHCK 132
      IF(.NOT.INCDEQ)  GO TO 44                                         SHCK 133
      WRITE (6,862)                                                     SHCK 134
  862 FORMAT (1H ,35X,55HEQUILIBRIUM COMPOSITION FOR INCIDENT SHOCKED COSHCK 135
     1NDITIONS //)                                                      SHCK 136
      GO TO 45                                                          SHCK 137
   44 WRITE (6,863)                                                     SHCK 138
  863 FORMAT (1H ,37X,50HFROZEN COMPOSITION FOR INCIDENT SHOCKED CONDITISHCK 139
     1ONS//)                                                            SHCK 140
   45 EQL = .FALSE.                                                     SHCK 141
      CALL OUT1                                                         SHCK 142
      WRITE(6,46)                                                       SHCK 143
   46 FORMAT (16H INITIAL GAS (1) )                                     SHCK 144
      FMT(4)=FMT13                                                      SHCK 145
      FMT(5)=FB                                                         SHCK 146
      FMT(7)=F4                                                         SHCK 147
      WRITE (6,FMT) FMA,FMB,FB,FB,(MACH1(J),J=1,NPT)                    SHCK 148
      FMT(7) = F2                                                       SHCK 149
      WRITE (6,FMT) FU1,FL(3),FL(4),FB,(U1(J),J=1,NPT)                  SHCK 150
      CALL OUT2                                                         SHCK 151
C                                                                       SHCK 152
C     BEGIN CALCULATIONS FOR 2ND CONDITION                              SHCK 153
C                                                                       SHCK 154
      IF(INCDEQ)  EQL=.TRUE.                                            SHCK 155
   47 NPT = 1                                                           SHCK 156
   48 GAMMA1 = GAMMAS(NPT)                                              SHCK 157
      UU = U1(NPT)                                                      SHCK 158
      M1 = WM(NPT)                                                      SHCK 159
      P1 = PPP(NPT)                                                     SHCK 160
      T1 = TTT(NPT)                                                     SHCK 161
      HS = HSUM(NPT)                                                    SHCK 162
      IF(REFL)  UU=U1U2(NPT)                                            SHCK 163
      MU12RT = M1*UU**2/(RR*T1)                                         SHCK 164
      IF(REFL)  GO TO 59                                                SHCK 165
      P21 = (2.*GAMMA1*MACH1(NPT)**2-GAMMA1+1.)/(GAMMA1+1.)             SHCK 166
      T21 = P21*(2./MACH1(NPT)**2+GAMMA1-1.)/(GAMMA1+1.)                SHCK 167
      IF((T1*T21).GT.2000..AND. EQL) T21 = .7*T21 + 600./T1             SHCK 168
      GO TO 61                                                          SHCK 169
C                                                                       SHCK 170
C    REFLECTED--SUBSCRIPTS 2=1, 5=2, P52=P21                            SHCK 171
C                                                                       SHCK 172
   59 T21 = 2.                                                          SHCK 173
      B2 = (-1.-MU12RT-T21)/2.                                          SHCK 174
      P21 = -B2+SQRT(B2**2-T21)                                         SHCK 175
   61 P21L=ALOG(P21)                                                    SHCK 176
      T21L=ALOG(T21)                                                    SHCK 177
      DO 100 ITR=1,8                                                    SHCK 178
      IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  WRITE(6,152) ITR,IT2,IT1,T21,  SHCK 179
     1IT2,IT1,P21                                                       SHCK 180
```


C-2

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  152 FORMAT(10HOITR NO.= ,I1,7X,1HT,I1,2H/T,I1,2H =,F9.4,7X,1HP,I1,2H/PSHCK 181
     1,I1,2H =,F9.4 )                                                   SHCK 182
      TT=T21*T1                                                         SHCK 183
      PP=P21*P1                                                         SHCK 184
      IF (.NOT.EQL) GO TO 40                                            SHCK 185
      CALL EQLBRM                                                       SHCK 186
      IF(TT.EQ.0.)  GO TO 430                                           SHCK 187
      GO TO 50                                                          SHCK 188
C                                                                       SHCK 189
C  FROZEN                                                               SHCK 190
C                                                                       SHCK 191
   40 TLN = ALOG (TT)                                                   SHCK 192
      IF(.NOT.INCDEQ)  GO TO 88                                         SHCK 193
      JS1 = 1                                                           SHCK 194
      CALL CPHS                                                         SHCK 195
      CPR(NPT) = CPSUM                                                  SHCK 196
      HSUM(NPT) = 0.                                                    SHCK 197
      DO 84  J= 1,NS                                                    SHCK 198
      IF(IUSE(J).EQ.0)  HSUM(NPT)=HSUM(NPT)+HO(J)*EN(J,NPT)             SHCK 199
   84 CONTINUE                                                          SHCK 200
      HSUM(NPT) = HSUM(NPT)*TT                                          SHCK 201
      GO TO 50                                                          SHCK 202
   88 CALL HCALC                                                        SHCK 203
      IF(TT.EQ.0.)  GO TO 150                                           SHCK 204
      HSUM(NPT) = HSUBO                                                 SHCK 205
      CPR(NPT) = CPR1                                                   SHCK 206
C                                                                       SHCK 207
   50 RHO12 = M1*T21/(WM(NPT)*P21)                                      SHCK 208
      GG=RHO12*MU12RT                                                   SHCK 209
      RHO52 = 1./RHO12                                                  SHCK 210
      IF(REFL)  GG=-MU12RT*RHO52/(RHO52-1.)**2                          SHCK 211
      G(1,1)=-GG*DLVPT(NPT)-P21                                         SHCK 212
      G(1,2)=-GG*DLVTP(NPT)                                             SHCK 213
      G(1,3)=P21-1.+GG-MU12RT                                           SHCK 214
      IF(REFL)  G(1,3) = P21-1.+GG*(RHO52-1.)                           SHCK 215
      GG = GG*T1/M1                                                     SHCK 216
      IF(.NOT.REFL)  GG=GG*RHO12                                        SHCK 217
      G(2,1)=-GG*DLVPT(NPT)+TT*(DLVTP(NPT)-1.)/WM(NPT)                  SHCK 218
      G(2,2)=-GG*DLVTP(NPT)-TT*CPR(NPT)                                 SHCK 219
      GG = 1.-RHO12**2                                                  SHCK 220
      IF(REFL)  GG=(RHO52+1.)/(RHO52-1.)                                SHCK 221
      G(2,3)=HSUM(NPT)-HS-UU**2*GG/(2.*RR)                              SHCK 222
      X(3)=G(1,1)*G(2,2)-G(1,2)*G(2,1)                                  SHCK 223
      X(1)=(G(1,3)*G(2,2)-G(2,3)*G(1,2))/X(3)                           SHCK 224
      X(2)=(G(1,1)*G(2,3)-G(2,1)*G(1,3))/X(3)                           SHCK 225
C                                                                       SHCK 226
      AX = X(1)                                                         SHCK 227
      AXX = X(2)                                                        SHCK 228
      IF(AX.LT.0.) AX = -AX                                             SHCK 229
      IF (AXX.LT.0.) AXX = -AXX                                         SHCK 230
      IF (AXX.GT.AX)  AX = AXX                                          SHCK 231
      IF(AX.LT..00005)  GO TO 150                                       SHCK 232
      AX = AX/.4C54652                                                  SHCK 233
      IF(AX.LE.1.)  GO TO 75                                            SHCK 234
      X(1) = X(1)/AX                                                    SHCK 235
      X(2) = X(2)/AX                                                    SHCK 236
   75 P21L=P21L+X(1)                                                    SHCK 237
      T21L=T21L+X(2)                                                    SHCK 238
      P21=EXP(P21L)                                                     SHCK 239
      T21=EXP(T21L)                                                     SHCK 240
  100 CONTINUE                                                          SHCK 241
      WRITE(6,125) U1(NPT)                                              SHCK 242
  125 FORMAT(25HODID NOT CONVERGE FOR U1=,F8.2,56H   ANSWERS PROBABLY NOSHCK 243
     1T RELIABLE, SOLUTION MAY NOT EXIST)                               SHCK 244
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```
  150 RRHO(NPT) = RHO52                                                    SHCK 245
      M2M1(NPT) = WM(NPT)/M1                                               SHCK 246
      PCP(NPT) = P21                                                       SHCK 247
      T2T1(NPT) = T21                                                      SHCK 248
      UTWO(NPT) = UU*RHO12                                                 SHCK 249
      U1U2(NPT) = UU-UTWO(NPT)                                             SHCK 250
      IF(TT.GE.TLOW/1.5.AND.TT.LE.THIGH*1.25)  GO TO 153                   SHCK 251
      WRITE(6,1152)                                                        SHCK 252
 1152 FORMAT(47HOTEMPERATURE IS OUT OF RANGE OF THE THERMO DATA)           SHCK 253
  153 IF(.NOT.REFL)  GO TO 154                                             SHCK 254
      U5(NPT) = UU/(RHO52-1.)                                              SHCK 255
      U2STAR(NPT) = U5(NPT)+UU                                             SHCK 256
  154 IF(EQL)  GO TO 431                                                   SHCK 257
C                                                                          SHCK 258
C  FROZEN                                                                  SHCK 259
C                                                                          SHCK 260
  161 PPP(NPT) = PP                                                        SHCK 261
      TTT(NPT) = TT                                                        SHCK 262
      GAMMAS(NPT) = CPR(NPT)/(CPR(NPT)-1./M1)                              SHCK 263
      VLM(NPT) = RR*TT/(M1*101.325*PP)                                     SHCK 264
      IF(.NOT.INCOEQ)  GO TO 431                                           SHCK 265
      SSUM(NPT) = 0.                                                       SHCK 266
      DO 166  J=1,NS                                                       SHCK 267
      PMN = PP*M1*EN(J,NPT)                                                SHCK 268
      IF(IUSE(J).EQ.0) SSUM(NPT)=SSUM(NPT)+EN(J,NPT)*(S(J)-ALOG(PMN))      SHCK 269
  166 CONTINUE                                                             SHCK 270
C                                                                          SHCK 271
      GO TO 431                                                            SHCK 272
  430 IF(NPT.LT.1)  GO TO 1000                                             SHCK 273
      NSK = NPT                                                            SHCK 274
C                                                                          SHCK 275
  431 ISV = 0                                                              SHCK 276
      IF(NPT.LT.NSK)  ISV=NPT                                              SHCK 277
      IF(NPT.EQ.1)  ISV=-1                                                 SHCK 278
      NPT = NPT+1                                                          SHCK 279
      IF(EQL)  CALL SAVE                                                   SHCK 280
      IF(NPT.LE.NSK)  GO TO 48                                             SHCK 281
      NPT = NSK                                                            SHCK 282
C                                                                          SHCK 283
C  OUTPUT--2ND CONDITION                                                   SHCK 284
C                                                                          SHCK 285
      WRITE(6,156)                                                         SHCK 286
  156 FORMAT(1H )                                                          SHCK 287
      IF(REFL)  GO TO 56                                                   SHCK 288
      IF(.NOT.EQL)  WRITE(6,57)                                            SHCK 289
   57 FORMAT(34HOSHOCKED GAS (2)--INCIDENT--FROZEN)                        SHCK 290
      IF(EQL)  WRITE(6,157)                                                SHCK 291
  157 FORMAT(39HOSHOCKED GAS (2)--INCIDENT--EQUILIBRIUM)                   SHCK 292
      DO 55  I=1,4                                                         SHCK 293
   55 W(I) = FV2(I)                                                        SHCK 294
      W(5) = FPP                                                           SHCK 295
      W(6) = ONE                                                           SHCK 296
      W(7) = FTT                                                           SHCK 297
      W(8) = FMM                                                           SHCK 298
      W(9) = FRA                                                           SHCK 299
      W(10) = FU2                                                          SHCK 300
      GO TO 700                                                            SHCK 301
   56 IF(.NOT.EQL)  WRITE(6,58)                                            SHCK 302
      IF(EQL)  WRITE(6,690)                                                SHCK 303
   58 FORMAT(35HOSHOCKED GAS (5)--REFLECTED--FROZEN)                       SHCK 304
  690 FORMAT(40HOSHOCKED GAS (5)--REFLECTED--EQUILIBRIUM)                  SHCK 305
      DO 65  I=1,4                                                         SHCK 306
   65 W(I) = FUV(I)                                                        SHCK 307
      W(5) = FP5                                                           SHCK 308
      W(6) = TWO                                                           SHCK 309
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      W(7) = FT5                                                        SHCK 310
      W(8) = FM5                                                        SHCK 311
      W(9) = FR5                                                        SHCK 312
      W(10) = FU5                                                       SHCK 313
  700 FMT(7) = F2                                                       SHCK 314
      WRITE (6,FMT)W(10),FL(3),FL(4),FB,(UTWO(J),J=1,NPT)               SHCK 315
      CALL OUT2                                                         SHCK 316
      WRITE(6,156)                                                      SHCK 317
      FMT(7)=F3                                                         SHCK 318
      WRITE(6,FMT)W(5),W(6),FB,FB,(PCP(J),J=1,NPT)                      SHCK 319
      WRITE(6,FMT)W(7),W(6),FB,FB,(T2T1(J),J=1,NPT)                     SHCK 320
      FMT(7)=F4                                                         SHCK 321
      WRITE(6,FMT)W(8),W(6),FB,FB,(M2M1(J),J=1,NPT)                     SHCK 322
      WRITE(6,FMT)W(9),FRB,W(6),FB,(RRHO(J),J=1,NPT)                    SHCK 323
      FMT(7) = F2                                                       SHCK 324
      WRITE(6,FMT) (W(I),I=1,4),(U1U2(J),J=1,NPT)                       SHCK 325
      IF(.NOT.EQL)  GO TO 850                                           SHCK 326
      CALL OUT3                                                         SHCK 327
      GO TO 865                                                         SHCK 328
C                                                                       SHCK 329
C   WRITE FROZEN MOLE FRACTIONS                                         SHCK 330
C                                                                       SHCK 331
  850 FMT(7) = F5                                                       SHCK 332
      IF(.NOT.INCDEQ)  GO TO 852                                        SHCK 333
      EQL = .TRUE.                                                      SHCK 334
      CALL OUT3                                                         SHCK 335
      EQL = .FALSE.                                                     SHCK 336
      GO TO 865                                                         SHCK 337
  852 WRITE(6,854)                                                      SHCK 338
  854 FORMAT (15HOMOLE FRACTIONS //)                                    SHCK 339
      DO 856 N = 1, NREAC                                               SHCK 340
      J = NUM(N,5)                                                      SHCK 341
      DO 855 I = 1,NPT                                                  SHCK 342
      V(I) = EN(J,I)*M1                                                 SHCK 343
  855 CONTINUE                                                          SHCK 344
      WRITE (6,FMT) SUB (J,1),SUB(J,2),FB,FB,(V(I),I = 1,NPT)           SHCK 345
  856 CONTINUE                                                          SHCK 346
C                                                                       SHCK 347
  865 RETURN                                                            SHCK 348
C                                                                       SHCK 349
      ENTRY SHCK1                                                       SHCK 350
C                                                                       SHCK 351
      IF(.NOT.SREFL)  GO TO 948                                         SHCK 352
      IF(.NOT.REFL)  GO TO 935                                          SHCK 353
      IF(EQL.OR..NOT.REFLEQ)  GO TO 948                                 SHCK 354
      GO TO 940                                                         SHCK 355
  935 REFL = .TRUE.                                                     SHCK 356
      IT2 = 5                                                           SHCK 357
      IT1 = 2                                                           SHCK 358
      EQL = .TRUE.                                                      SHCK 359
      IF(.NOT.REFLFZ)  GO TO 47                                         SHCK 360
      EQL = .FALSE.                                                     SHCK 361
      IF(.NOT.REFLEQ)  GO TO 47                                         SHCK 362
      J = 0                                                             SHCK 363
      DO 936  I=1,NPT                                                   SHCK 364
      J = J+1                                                           SHCK 365
      SG(J) = U1U2(I)                                                   SHCK 366
      J = J+1                                                           SHCK 367
      SG(J)   = WM(I)                                                   SHCK 368
      J = J+1                                                           SHCK 369
      SG(J)   = PPP(I)                                                  SHCK 370
      J = J+1                                                           SHCK 371
      SG(J)   = TTT(I)                                                  SHCK 372
      J = J+1                                                           SHCK 373
      SG(J)   = HSUM(I)                                                 SHCK 374
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      J = J+1                                                          SHCK 375
      SG(J) = GAMMAS(I)                                                SHCK 376
  936 CONTINUE                                                         SHCK 377
      GO TO 47                                                         SHCK 378
  940 J = 1                                                            SHCK 379
      DO 946  I=1,NPT                                                  SHCK 380
      U1U2(I) = SG(J)                                                  SHCK 381
      WM(I) = SG(J+1)                                                  SHCK 382
      PPP(I) = SG(J+2)                                                 SHCK 383
      TTT(I) = SG(J+3)                                                 SHCK 384
      HSUM(I) = SG(J+4)                                                SHCK 385
      GAMMAS(I) = SG(J+5)                                              SHCK 386
  946 J = J+6                                                          SHCK 387
      EQL = .TRUE.                                                     SHCK 388
      GO TO 47                                                         SHCK 389
  948 IF(.NOT.INCDEQ.OR..NOT.INCDFZ)  GO TO 950                        SHCK 390
      INCDEQ = .FALSE.                                                 SHCK 391
      EQL = .FALSE.                                                    SHCK 392
      GO TO 17                                                         SHCK 393
  950 IF(IOF.LT.NOF)  GO TO 21                                         SHCK 394
      TP = .FALSE.                                                     SHCK 395
      DO 999 N=1,NREAC                                                 SHCK 396
      RTEMP(N) = T(1)                                                  SHCK 397
  999 CONTINUE                                                         SHCK 398
 1000 RETURN 1                                                         SHCK 399
      END                                                              SHCK 400
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C
      SUBROUTINE DETON (*)                                             DETN   1
C                                                                      DETN   2
C     CHAPMAN-JOUGUET DETONATIONS                                      DETN   3
C                                                                      DETN   4
C  THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR     DETN   5
C     IBM 360 MACHINES ONLY                                            DETN   6
C                                                                      DETN   7
C     DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS                DETN   8
C     DOUBLE PRECISION COEF,S,EN,ENLN,HO,DELN                          DETN   9
C                                                                      DETN  10
      LOGICAL HP,SP,TP,EQL,TSCHED                                      DETN  11
C                                                                      DETN  12
      DIMENSION GM(13),CP(13),H1(13),PUB(13),TUB(13),GM1(13),RRHO(13)  DETN  13
C                                                                      DETN  14
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),    DETN  15
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13), DETN  16
     2 VLM(13),TCTN(13)                                                DETN  17
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), DETN  18
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)  DETN  19
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),RO(10),BOP(10,2),DETN  20
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      DETN  21
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         DETN  22
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FCX(15),DENS(15),DETN  23
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      DETN  24
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   DETN  25
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, DETN  26
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, DETN  27
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            DETN  28
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        DETN  29
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       DETN  30
     2 APPL,ARATIO,ELN                                                 DETN  31
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      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),    DETN  32
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2,          DETN  33
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                          DETN  34
C                                                                        DETN  35
      EQUIVALENCE(CP,DATA),(GM,SPIM),(H1,VACI),(PUB,SUBAR),(TUB,SUPAR)   DETN  36
      EQUIVALENCE(GM1,AEAT),(K,ISV)                                      DETN  37
      EQUIVALENCE(AM1,DATA(20)), (CPR1,DATA(21))                         DETN  38
C                                                                        DETN  39
      DATA FT1/4HT1,D/, FP1/4HP1,A/, FH1/4HH1,C/, FM1/4HM1,M/            DETN  40
     1              , FG1/4HA1  /, FPP/4HP/P1/, FTT/4HT/T1/              DETN  41
     2 ,   FUD/4HDET /, FMM/4HM/M1/, FRA/4HRHO//, FRB/4HRHO1/           DETN  42
     3 ,   FMA/4HMACH/, FMB/4H NO./, IZERO/2H0C/                        DETN  43
C                                                                        DETN  44
      IOF = 0                                                            DETN  45
C                                                                        DETN  46
C     IF NO T SCHEDULE, SET TSCHED=.FALSE. AND USE T FROM FIRST REACTANT DETN  47
C                                                                        DETN  48
      TSCHED = .TRUE.                                                    DETN  49
      IF(T(1).NE.0.)  GO TO 3                                            DETN  50
      T(1) = RTEMP(1)                                                    DETN  51
      TSCHED = .FALSE.                                                   DETN  52
      GO TO 7                                                            DETN  53
    3 DO 4  N=1,NREAC                                                    DETN  54
      NAME(N,5) = IZERO                                                  DETN  55
    4 CONTINUE                                                           DETN  56
    7 TT = T(1)                                                          DETN  57
      IOF = IOF+1                                                        DETN  58
      OF = OXF(IOF)                                                      DETN  59
      CALL NEWOF                                                         DETN  60
      WRITE (6,11)                                                       DETN  61
   11 FORMAT(33H1DETONATION VELOCITY CALCULATIONS)                       DETN  62
C                                                                        DETN  63
C     BEGIN T LOOP.                                                      DETN  64
C                                                                        DETN  65
      IT = 0                                                             DETN  66
  901 IT = IT + 1                                                        DETN  67
      T1= T(IT)                                                          DETN  68
      TT = T1                                                            DETN  69
      IF(.NOT.TSCHED)  GO TO 20                                          DETN  70
      CALL HCALC                                                         DETN  71
      IF(TT.EQ.0.)  RETURN 1                                             DETN  72
   20 IF(IDEBUG.NE.0)  CALL OUT1                                         DETN  73
C                                                                        DETN  74
C     BEGIN P LOOP.                                                      DETN  75
C                                                                        DETN  76
      IP = 0                                                             DETN  77
  903 IP =IP + 1                                                         DETN  78
      P1= P(IP)                                                          DETN  79
      H1(NPT) = HSUB0*R                                                  DETN  80
      TUB(NPT)=T1                                                        DETN  81
      PUB(NPT)=P1                                                        DETN  82
      CP(NPT) = CPR1*R                                                   DETN  83
      ITR= 0                                                             DETN  84
      TT= 3800.                                                          DETN  85
      PP1= 15.                                                           DETN  86
      PP= PP1*P1                                                         DETN  87
C                                                                        DETN  88
C     CALCULATE ENTHALPY FOR INITIAL ESTIMATE OF T2(TT AFTER EQLBRM)     DETN  89
C                                                                        DETN  90
      HSUB0 = H1(NPT)/R + .75*T1*PP1/AM1                                 DETN  91
      TP = .FALSE.                                                       DETN  92
      HP= .TRUE.                                                         DETN  93
      CALL EQLBRM                                                        DETN  94
      HSUB0 = H1(NPT)/R                                                  DETN  95
      HP= .FALSE.                                                        DETN  96
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      IF(TT.EQ.0.)  GO TO 902                                                DETN  97
      GAM= GAMMAS(NPT)                                                       DETN  98
      TT1= TT/T1                                                             DETN  99
      II= 0                                                                  DETN 100
      TEM=TT1-.75*PP1/(CPR(NPT)*AM1)                                         DETN 101
      AMM=WM(NPT)/AM1                                                        DETN 102
      WRITE(6,190)TT                                                         DETN 103
  190 FORMAT(8HOT EST.=,F8.2/11X,4HP/P1,17X,4HT/T1)                          DETN 104
      WRITE(6,203) II,PP1,TT1                                                DETN 105
C                                                                            DETN 106
C     LOOP FOR IMPROVING T2/T1 AND P2/P1 INITIAL ESTIMATE.                   DETN 107
C                                                                            DETN 108
  200 DO 202 II=1,3                                                          DETN 109
      ALFA=AMM/TT1                                                           DETN 110
      PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA)      DETN 111
      RK=PP1*ALFA                                                            DETN 112
      TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)                       DETN 113
      IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  WRITE(6,203) II,PP1,TT1             DETN 114
  203 FORMAT (I5,2E20.8)                                                     DETN 115
  202 CONTINUE                                                               DETN 116
      TP= .TRUE.                                                             DETN 117
      TT= T1*TT1                                                             DETN 118
      RR1 = PP1*AMM/TT1                                                      DETN 119
C                                                                            DETN 120
C     BEGIN MAIN ITERATION LOOP.                                             DETN 121
C                                                                            DETN 122
  205 ITR= ITR+1                                                             DETN 123
      PP= P1*PP1                                                             DETN 124
      CALL EQLBRM                                                            DETN 125
      IF (NPT.EQ.0) GO TO 1000                                               DETN 126
      IF (TT.EQ.0.) GO TO 860                                                DETN 127
      GAM= GAMMAS(NPT)                                                       DETN 128
      AMM= WM(NPT)/AM1                                                       DETN 129
      RR1= PP1*AMM/TT1                                                       DETN 130
      A11= 1./PP1 + GAM*RR1*DLVPT(NPT)                                       DETN 131
      A12= GAM*RR1*DLVTP(NPT)                                                DETN 132
      A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.           DETN 133
      A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)                    DETN 134
      B1= 1./PP1-1.+GAM*(RR1-1.)                                             DETN 135
      B2= WM(NPT)*(HSUM(NPT)-H1(NPT)/R)/TT-.5*GAM*(RR1*RR1-1.)               DETN 136
      D = A11*A22-A12*A21                                                    DETN 137
      X1 = (A22*B1-A12*B2)/D                                                 DETN 138
      X2 = (A11*B2-A21*B1)/D                                                 DETN 139
      ALAM= 1.                                                               DETN 140
      TEM = X1                                                               DETN 141
      IF(TEM.LT.0.)  TEM = -TEM                                              DETN 142
      IF(X2.GT.TEM)  TEM=X2                                                  DETN 143
      IF (-X2.GT.TEM) TEM = -X2                                              DETN 144
      IF(TEM.GT.0.4054652)  ALAM=.4054652/TEM                                DETN 145
      PP1= PP1*EXP(X1*ALAM)                                                  DETN 146
      TT1= TT1*EXP(X2*ALAM)                                                  DETN 147
      TT = T1*TT1                                                            DETN 148
      UD = RR1*(RR*GAM*TT/WM(NPT))**.5                                       DETN 149
      IF(IDEBUG.GT.0.AND.NPT.GE.IDEBUG)  WRITE(6,30)ITR,PP1,TT1,RR1,X1,      DETN 150
     1X2                                                                     DETN 151
   30 FORMAT(7HOITER =,I2,5X,6HP/P1 =,E15.8,5X,6HT/T1 =,E15.8,5X,10HRHO/     DETN 152
     1RHO1 =,E15.8/7X,13HDEL LN P/P1 =,E15.8,5X,13HDEL LN T/T1 =,E15.8)      DETN 153
C                                                                            DETN 154
C     CONVERGENCE TEST                                                       DETN 155
C                                                                            DETN 156
      IF(ITR.LT.8.AND.TEM.GT.0.5E-04)  GO TO 205                             DETN 157
      IF(ITR.LT.8)  GO TO 35                                                 DETN 158
      WRITE(6,34)                                                            DETN 159
   34 FORMAT(53HOCONSERVATION EQNS WERE NOT SATISFIED IN 8 ITERATIONS)       DETN 160
      NPT = NPT-1                                                            DETN 161
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      TT = 0.                                                          DETN 162
      GO TO 150                                                        DETN 163
   35 RRHO(NPT)=RR1                                                    DETN 164
      IF (CP(NPT).EQ.0.) GO TO 40                                      DETN 165
      GM1(NPT) = CP(NPT) /(CP(NPT)-R/AM1)                              DETN 166
      VMOC(NPT) = UD/(RR*GM1(NPT)*T1/AM1)**.5                          DETN 167
      GO TO 150                                                        DETN 168
   40 GM1(NPT) = 0.                                                    DETN 169
      VMOC(NPT) = 0.                                                   DETN 170
  150 K = 0                                                            DETN 171
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860                 DETN 172
      K = NPT                                                          DETN 173
      IF(NPT.NE.13)  GO TO 870                                         DETN 174
C                                                                      DETN 175
C  OUTPUT                                                              DETN 176
C                                                                      DETN 177
  860 WRITE (6,5)                                                      DETN 178
    5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )DETN 179
      CALL OUT1                                                        DETN 180
      WRITE(6,46)                                                      DETN 181
   46 FORMAT(13H UNBURNED GAS//)                                       DETN 182
      FMT(4)=FMT13                                                     DETN 183
      FMT(5)=F8                                                        DETN 184
      FMT(7)=F4                                                        DETN 185
      WRITE(6,FMT)  FP1,FP(2),FB,FB,(PUB(J),J=1,NPT)                   DETN 186
      FMT(7)=F2                                                        DETN 187
      WRITE(6,FMT)  FT1,FT(2),FB,FB,(TUB(J),J=1,NPT)                   DETN 188
      WRITE(6,FMT)  FH1,FH(2),FB,FB,(H1(J), J=1,NPT)                   DETN 189
      DO 56 I=1,NPT                                                    DETN 190
      V(I)=AM1                                                         DETN 191
      SONVEL(I) = (RR*GM1(I)*TUB(I)/AM1)**.5                           DETN 192
   56 CONTINUE                                                         DETN 193
      FMT(7)=F3                                                        DETN 194
      WRITE(6,FMT) FM1,FM(2),FM(3),FB,(V(J),J=1,NPT)                   DETN 195
      FMT(7)=F4                                                        DETN 196
      IF(.NOT.TSCHED)  GO TO 57                                        DETN 197
      WRITE(6,FMT)  FG(1),FG1,FB,FB,(GM1(J),J=1,NPT)                   DETN 198
      FMT(7)=F1                                                        DETN 199
      WRITE(6,FMT)  (FL(I),I=1,4),(SONVEL(J),J=1,NPT)                  DETN 200
   57 WRITE(6,58)                                                      DETN 201
   58 FORMAT(11HOBURNED GAS//)                                         DETN 202
      FMT(4)=FMT(6)                                                    DETN 203
      CALL OUT2                                                        DETN 204
      WRITE(6,68)                                                      DETN 205
   68 FORMAT(22HODETONATION PARAMETERS //)                             DETN 206
      FMT(7)=F3                                                        DETN 207
      DO 70 I=1,NPT                                                    DETN 208
      V(I)= PPP(I)/PUB(I)                                              DETN 209
      PCP(I)=TTT(I)/TUB(I)                                             DETN 210
      SONVEL(I)=SONVEL(I)*RRHO(I)                                      DETN 211
   70 CONTINUE                                                         DETN 212
      WRITE(6,FMT)  FPP,FB,FB,FB,(V(J),J=1,NPT)                        DETN 213
      WRITE(6,FMT)  FTT,FB,FB,FB,(PCP(J),J=1,NPT)                      DETN 214
      DO 73 I=1,NPT                                                    DETN 215
      V(I)=WM(I)/AM1                                                   DETN 216
   73 CONTINUE                                                         DETN 217
      FMT(7)=F4                                                        DETN 218
      WRITE(6,FMT)  FMM,FB,FB,FB,(V(J),J=1,NPT)                        DETN 219
      WRITE(6,FMT)  FRA,FRB,FB,FB,(RRHO(J),J=1,NPT)                    DETN 220
      IF(TSCHED)  WRITE(6,FMT) FMA,FMB,FB,FB,(VMOC(J),J=1,NPT)         DETN 221
      FMT(7)=F1                                                        DETN 222
      WRITE(6,FMT) FUD,FL(2),FL(3),FL(4),(SONVEL(J),J=1,NPT)           DETN 223
      EQL=.TRUE.                                                       DETN 224
      CALL OUT3                                                        DETN 225
C                                                                      DETN 226
C     END OUTPUT.                                                      DETN 227
```

```
C                                                                       DETN 228
      RETURN                                                            DETN 229
C                                                                       DETN 230
      ENTRY DETON1                                                      DETN 231
C                                                                       DETN 232
  865 IF(K.EQ.0.AND.IOF.EQ.NOF)  GO TO 1000                             DETN 233
      IF (NP.EQ.1 .AND. NT.EQ.1) GO TO 7                                DETN 234
      IDEBUG = IDEBUG-13                                                DETN 235
      WRITE(6,868)                                                      DETN 236
  868 FORMAT(1H1)                                                       DETN 237
      NPT = 0                                                           DETN 238
  870 NPT = NPT + 1                                                     DETN 239
      IF(ISV.EQ.1)  ISV=-1                                              DETN 240
      CALL SAVE                                                         DETN 241
      IF(IP.LT.NP) GO TO 903                                            DETN 242
  902 IF(IT.LT.NT) GO TO 901                                            DETN 243
      IF(IOF.GE.NOF)  GO TO 1000                                        DETN 244
      IDEBUG = IDEBUG+13                                                DETN 245
      GO TO 7                                                           DETN 246
 1000 IP = .FALSE.                                                      DETN 247
      RETURN 1                                                          DETN 248
      END                                                               DETN 249
```

```
C                                                                       BLOK   1
      BLOCK DATA                                                        BLOK   2
C                                                                       BLOK   3
      DIMENSION ATEM(3,50)                                              BLOK   4
C                                                                       BLOK   5
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),BLOK   6
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      BLOK   7
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         BLOK   8
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),BLOK   9
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      BLOK  10
      COMMON /OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4),   BLOK  11
     1 FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2,         BLOK  12
     2 FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                         BLOK  13
C                                                                       BLOK  14
      EQUIVALENCE (ATOM(1,52),ATEM)                                     BLOK  15
C                                                                       BLOK  16
C  ATOMIC SYMBOLS, WEIGHTS, AND VALENCES                                BLOK  17
C                                                                       BLOK  18
      DATA ATOM/ 2HE ,5.48597E-4,-1.,                                   BLOK  19
     A   2HH , 1.00797, 1.,   2HHE,  4.0026, 0.,   2HLI,  6.939  , 1., BLOK  20
     B   2HBE,  9.0122 , 2.,   2HB , 10.811 , 3.,   2HC , 12.01115, 4., BLOK  21
     C   2HN , 14.0067 , 0.,   2HO , 15.9994,-2.,   2HF , 18.9984 ,-1., BLOK  22
     D   2HNE, 20.183  , 0.,   2HNA, 22.9898, 1.,   2HMG, 24.312  , 2., BLOK  23
     E   2HAL, 26.9815 , 3.,   2HSI, 28.086 , 4.,   2HP , 30.9738 , 5., BLOK  24
     F   2HS , 32.064  , 4.,   2HCL, 35.453 ,-1.,   2HAR, 39.948  , 0., BLOK  25
     G   2HK , 39.102  , 1.,   2HCA, 40.080 , 2.,   2HSC, 44.956  , 3., BLOK  26
     H   2HTI, 47.900  , 4.,   2HV , 50.942 , 5.,   2HCR, 51.996  , 3., BLOK  27
     I   2HMN, 54.9380 , 2.,   2HFE, 55.847 , 3.,   2HCO, 58.9332 , 2., BLOK  28
     J   2HNI, 58.710  , 2.,   2HCU, 63.540 , 2.,   2HZN, 65.370  , 2., BLOK  29
     K   2HGA, 69.720  , 3.,   2HGE, 72.590 , 4.,   2HAS, 74.9216 , 3., BLOK  30
     L   2HSE, 78.960  , 4.,   2HBR, 79.909 ,-1.,   2HKR, 83.800  , 0., BLOK  31
     M   2HRB, 85.47   , 1.,   2HSR, 87.620 , 2.,   2HY , 88.905  , 3., BLOK  32
     N   2HZR, 91.220  , 4.,   2HNB, 92.906 , 5.,   2HMO, 95.94   , 6., BLOK  33
     O   2HTC, 99.000  , 7.,   2HRU,101.070 , 3.,   2HRH,102.905  , 3., BLOK  34
     P   2HPD,106.400  , 2.,   2HAG,107.870 , 1.,   2HCD,112.400  , 2., BLOK  35
     Q   2HIN,114.820  , 3.,   2HSN,118.690 , 4.,   2HSB,121.750  , 3. /BLOK  36
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```
      DATA ATEM/                                                                BLOK  36
     R    2HTE,127.600  , 4.,   2HI ,126.9044,-1.,   2HXE,131.300  , 0., BLOK  37
     S    2HCS,132.905  , 1.,   2HBA,137.340 , 2.,   2HLA,138.910  , 3., BLOK  38
     T    2HCE,140.120  , 3.,   2HPR,140.907 , 3.,   2HND,144.240  , 3., BLOK  39
     U    2HPM,145.000  , 3.,   2HSM,150.350 , 3.,   2HEU,151.960  , 3., BLOK  40
     V    2HGD,157.250  , 3.,   2HTB,158.924 , 3.,   2HDY,162.500  , 3., BLOK  41
     W    2HHO,164.930  , 3.,   2HER,167.260 , 3.,   2HTM,168.934  , 3., BLOK  42
     X    2HYB,173.040  , 3.,   2HLU,174.997 , 3.,   2HHF,178.490  , 4., BLOK  43
     Y    2HTA,180.948  , 5.,   2HW ,183.850 , 6.,   2HRE,186.200  , 7., BLOK  44
     Z    2HOS,190.200  , 4.,   2HIR,192.200 , 4.,   2HPT,195.090  , 4., BLOK  45
     A    2HAU,196.967  , 3.,   2HHG,200.590 , 2.,   2HTL,204.370  , 1., BLOK  46
     B    2HPB,207.190  , 2.,   2HBI,208.980 , 3.,   2HPO,210.000  , 2., BLOK  47
     C    2HAT,210.000  , 0.,   2HRN,222.000 , 0.,   2HFR,223.000  , 1., BLOK  48
     D    2HRA,226.000  , 2.,   2HAC,227.000 , 3.,   2HTH,232.038  , 4., BLOK  49
     E    2HPA,231.000  , 5.,   2HU ,238.030 , 6.,   2HNP,237.000  , 5., BLOK  50
     F    2HPU,242.000  , 4.,   2HAM,243.000 , 3.,   2HCM,247.000  , 3., BLOK  51
     G    2HBK,249.000  , 3.,   2HCF,251.000 , 3.,   2HES,254.000  , 0., BLOK  52
     H    2HD ,2.014102, 1./                                                   BLOK  53
C                                                                              BLOK  54
C     INFORMATION USED IN VARIABLE OUTPUT FORMAT                               BLOK  55
C                                                                              BLOK  56
      DATA FMT/3H(1H,4H,3A4,4H,A2,,3HF9.,2HO,,3HF9.,2HO,,3HF9.,2HO,,3HF9BLOK  57
     1.,2HO,,3HF9.,2HO,,3HF9.,2HO,,3HF9.,2HO,,3HF9.,2HO,,3HF9.,2HO,,3HF9BLOK  58
     2.,2HO,,3HF9.,2HO,,3HF9.,2HO,,3HF9.,1HO,1H)/, FB,F0,F1,F2,F3,F4,F5/BLOK  59
     31H  ,2HO,,2H1,,2H2,,2H3,,2H4,,2H5,/,FMT13/2H13/,FMT9X/3H9X,/,FMTI9BLOK  60
     4/3HI9,/                                                                 BLOK  61
      DATA                              FP/4HP, A,4HTM  ,2H  ,1H /             BLOK  62
     1,FT/4HT, D,4HEG K,4H    ,2H  /,FH/4HH, C,4HAL/G,2H  ,1H /               BLOK  63
     2,FS/4HS, C,4HAL/(,4HG)(K,2H) /,FM/4HM, M,4HOL W,2HT ,1H /               BLOK  64
     3,FV/4H(DLV,4H/DLF,4H)T  ,2H  /,FD/4H(DLV,4H/DLT,2H)P,1H /               BLOK  65
     4,FC/4HCP, ,4HCAL/,4H(G)(,2HK)/,FG/4HGAMM,4HA (S,2H) ,1H /               BLOK  66
     5,FL/4HSON ,4HVEL,,4HM/SE,2HC /                                          BLOK  67
C                                                                              BLOK  68
C     INFORMATION USED IN PERFORMANCE OUTPUT                                   BLOK  69
C                                                                              BLOK  70
      DATA FR1/4HPC/P/, FC1/2HCF/,     FN/4HMACH,4H NUM,4HBER ,1H /            BLOK  71
     1,FR/4HCSTA,4HR, F,4HT/SE,2HC  /,FI/4HISP,,4H LB-,4HSEC/,2HLB/           BLOK  72
     2,FA/4HIVAC,4H,LB-,4HSEC/,2HLB /,FA1/4HAE/A/,FA2/1HT/                    BLOK  73
      END                                                                      BLOK  74
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C
      SUBROUTINE TRANSP                                                        TRAN   1
C                                                                              TRAN   2
C     CALCULATES GAS TRANSPORT PROPERTIES                                      TRAN   3
C                                                                              TRAN   4
C     MAXIMUM = 20 MOLECULES AND 17 REACTIONS                                  TRAN   5
C     NUMBER OF MOLECULES = NM                                                 TRAN   6
C     NUMBER OF CHEMICAL REACTIONS = NR                                        TRAN   7
C     IF PUNCHED CARDS WANTED, PUNCH = TRUE                                    TRAN   8
C     ARRAY OF STOICHIOMETRIC COEFFICIENTS = STC                               TRAN   9
C     NUMBER OF ROTATIONAL MODES = ROTM                                        TRAN  10
C     ROTATIONAL COLLISION NUMBER = ZROT                                       TRAN  11
C     VIBRATIONAL COLLISION NUMBER = ZVIB                                      TRAN  12
C     VIBRATIONAL HEAT CAPACITY = CVIBR                                        TRAN  13
C     MAXIMUM = 120 TABLES OF 20 TEMPERATURES EACH                             TRAN  14
C     IF CROSS SECTION DATA NTAB = 1 , IF RELAXATION DATA NTAB = 2             TRAN  15
C     VISCOSITY=ANS(1), MONATOMIC CONDUCTIVITY= ANS(2),                        TRAN  16
C     INTERNAL CONDUCTIVITY=ANS(3), FROZEN CONDUCTIVITY=ANS(4),                TRAN  17
C     REACTION CONDUCTIVITY=ANS(5), EQUILIBRIUM CONDUCTIVITY=ANS(6),           TRAN  18
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C      FROZEN CP=ANS(7), EQUILIBRIUM CP=ANS(8),                                  TRAN  19
C      FROZEN PRANDTL NUMBER=ANS(9), EQUILIBRIUM PRANDTL NUMBER=ANS(10),         TRAN  20
C      LEWIS NUMBER=ANS(11), MOLECULAR WEIGHT=ANS(12), DENSITY=ANS(13),          TRAN  21
C      REACTION CP=ANS(14), ENTHALPY=ANS(15)                                     TRAN  22
C                                                                                TRAN  23
       DOUBLE PRECISION G,X,GMAT,CHECK,SUM1,SUM2                                 TRAN  24
       INTEGER SUB,SPECIE,SPECE                                                  TRAN  25
       REAL MONCON,INTCON,LEWIS                                                  TRAN  26
       LOGICAL TRNSPT,FROZN,PUNCH,NODATA                                         TRAN  27
C                                                                                TRAN  28
       COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),             TRAN  29
      1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),          TRAN  30
      2 VLM(13),TOTN(13)                                                         TRAN  31
       COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100),         TRAN  32
      1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)           TRAN  33
       COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),        TRAN  34
      1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),              TRAN  35
      2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),                 TRAN  36
      3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),        TRAN  37
      4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)              TRAN  38
       COMMON /DOUBLE/ G(20,21), X(20)                                           TRAN  39
       COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,           TRAN  40
      1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK,        TRAN  41
      2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV,        TRAN  42
      3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT                   TRAN  43
       COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),                TRAN  44
      1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,               TRAN  45
      2 APPL,ARATIO,ELN                                                          TRAN  46
       COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,           TRAN  47
      1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,                    TRAN  48
      2 FIRSTP,FIRSTV                                                            TRAN  49
       COMMON /TRANS/ TEM(100,20),TABLES(100,20,3),SPECIE(100,2,3),              TRAN  50
      1 OMEGA(20,20),ASTAR(20,20),BSTAR(20,20),CPRR(20),                         TRAN  51
      2 HRRT(20),ZROT(20),ZVIB(20),CVIBR(20),ROTM(20),RELXTN(20),                TRAN  52
      3 ROTNM(80),STCF(17,20),STC(17,20),STCOEF(20),ANS(15),                     TRAN  53
      4 SPECE(2,3),NTT(100),NTAB(100),NR,N                                       TRAN  54
       COMMON /INTERP/ Z(20),Y(20,3),NTP,ANSR(3)                                 TRAN  55
       COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA                                  TRAN  56
C                                                                                TRAN  57
       DIMENSION ETA(20,20),DELH(17),CHECK(20)                                   TRAN  58
       DIMENSION GMAT(20,21),RTPD(20,20),STXS(20,20),XSKL(20,20)                 TRAN  59
C                                                                                TRAN  60
       EQUIVALENCE (ANS(1) ,VISC  ), (ANS(2) ,MONCON), (ANS(3) ,INTCON)          TRAN  61
       EQUIVALENCE (ANS(4) ,FRZCON), (ANS(5) ,REACON), (ANS(6) ,EQCON )          TRAN  62
       EQUIVALENCE (ANS(7) ,CPFROZ), (ANS(8) ,CPEQ  ), (ANS(9) ,PRFROZ)          TRAN  63
       EQUIVALENCE (ANS(10),PREQ  ), (ANS(11),LEWIS ), (ANS(12),WTMOL )          TRAN  64
       EQUIVALENCE (ANS(13),DENSTY), (ANS(14),CPREAC), (ANS(15),ENTLPY)          TRAN  65
       EQUIVALENCE (EQL,EQLB)      , (S,ETA)         , (RTPD,OMEGA)              TRAN  66
       EQUIVALENCE (STXS,BSTAR)    , (XSKL,ETA)                                  TRAN  67
C                                                                                TRAN  68
       DATA PI/3.14159265/,AVGDRO/6.022169/,BOLTZ/1.380622/                      TRAN  69
       DATA RPVT/82.0562/                                                        TRAN  70
       DATA ND/4HLAST/                                                           TRAN  71
C                                                                                TRAN  72
       NAMELIST /MATRX/GMAT                                                      TRAN  73
C                                                                                TRAN  74
C      READ TRANSPORT AND RELAXATION DATA FROM TAPE 3                            TRAN  75
C      SEARCH FOR AND STORE INTERACTIONS TO BE CONSIDERED                        TRAN  76
C                                                                                TRAN  77
       NK=1                                                                      TRAN  78
   12  READ(3) ((SPECE(I,L),L=1,3),I=1,2),NTP,NTB,ROTN                           TRAN  79
       IF(SPECE(1,1).EQ.ND) GO TO 10                                             TRAN  80
       K=1                                                                       TRAN  81
       DO 5 J=1,NS                                                               TRAN  82
       DO 1 N=1,NPT                                                              TRAN  83
       TESTEN=(1.E-7)/WM(N)                                                      TRAN  84
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     1 IF(EN(J,N).GT.TESTEN) GO TO 2                                          TRAN  85
       GO TO 5                                                                TRAN  86
     2 DO 4 I=1,3                                                             TRAN  87
     4 IF(SPECE(K,I).NE.SUB(J,I)) GO TO 5                                     TRAN  88
       GO TO 6                                                                TRAN  89
     5 CONTINUE                                                               TRAN  90
       READ(3) (TEM(NK,I),(TABLES(NK,I,L),L=1,3),I=1,NTP)                     TRAN  91
       GO TO 13                                                               TRAN  92
     6 K=2                                                                    TRAN  93
       DO 8 JJ=1,NS                                                           TRAN  94
       DO 7 II=1,3                                                            TRAN  95
     7 IF(SPECE(K,II).NE.SUB(JJ,II)) GO TO 8                                  TRAN  96
       IF(EN(JJ,N).GT.TESTEN) GO TO 10                                        TRAN  97
     8 CONTINUE                                                               TRAN  98
       READ(3) (TEM(NK,I),(TABLES(NK,I,L),L=1,3),I=1,NTP)                     TRAN  99
       GO TO 13                                                               TRAN 100
    10 DO 12 L=1,3                                                            TRAN 101
       DO 12 I=1,2                                                            TRAN 102
    12 SPECIE(NK,I,L)=SPECE(I,L)                                              TRAN 103
       IF(SPECIE(NK,1,1).EQ.ND) GO TO 17                                      TRAN 104
       NTT(NK)=NTP                                                            TRAN 105
       NTAB(NK)=NTB                                                           TRAN 106
       ROTNM(NK)=ROTN                                                         TRAN 107
       READ(3) (TEM(NK,I),(TABLES(NK,I,L),L=1,3),I=1,NTP)                     TRAN 108
       NK=NK+1                                                                TRAN 109
       IF(NK.GT.100) GO TO 19                                                 TRAN 110
       GO TO 13                                                               TRAN 111
    19 WRITE(6,18)                                                            TRAN 112
    18 FORMAT(1HO,40X,50HTABLES OF TRANSPORT AND RELAXATION DATA ARE FILLTRAN 113
      1ED)                                                                    TRAN 114
    17 REWIND 3                                                               TRAN 115
C                                                                             TRAN 116
C      START TRANSPORT CALCULATIONS                                           TRAN 117
C                                                                             TRAN 118
    23 DO 3 N=1,NPT                                                           TRAN 119
       IF(ISV.EQ.0.AND.MAXNP.GT.12) CALL OUT                                  TRAN 120
       IF(MAXNP.GT.51) CALL OUT                                               TRAN 121
       TT=TTT(N)                                                              TRAN 122
       PP=PPP(N)                                                              TRAN 123
C                                                                             TRAN 124
       CALL INPUT                                                             TRAN 125
C                                                                             TRAN 126
       K=1                                                                    TRAN 127
       IF(TT.LE.TMID) K=2                                                     TRAN 128
       DO 26 I=1,NM                                                           TRAN 129
       J=IND(I)                                                               TRAN 130
       CPRR(I)=(((COEF(K,5,J)*TT+COEF(K,4,J))*TT+COEF(K,3,J))*TT+             TRAN 131
      1 COEF(K,2,J))*TT+COEF(K,1,J)                                           TRAN 132
       HRRT(I) = ((((COEF(K,5,J)/5.)*TT+COEF(K,4,J)/4.)*TT+COEF(K,3,J)/      TRAN 133
      1 3.)*TT+COEF(K,2,J)/2.)*TT+COEF(K,1,J)+COEF(K,6,J)/TT                  TRAN 134
    26 CONTINUE                                                               TRAN 135
C                                                                             TRAN 136
C      CALCULATE VISCOSITY AND MONATOMIC THERMAL CONDUCTIVITY                 TRAN 137
C                                                                             TRAN 138
       CONST = (5./16.)*SQRT(1.0E5*BOLTZ/(PI*AVGDRO))                         TRAN 139
       DO 24 I=1,15                                                           TRAN 140
    24 ANS(I)=0.0                                                             TRAN 141
       DO 25 I=1,NM                                                           TRAN 142
       DO 25 J=I,NM                                                           TRAN 143
       ETA(I,J)= CONST*SQRT(2.0*WMOL(I)*WMOL(J)*TT/(WMOL(I)+WMOL(J)))/        TRAN 144
      1 OMEGA(I,J)                                                            TRAN 145
    25 ETA(J,I)=ETA(I,J)                                                      TRAN 146
       DO 27 I=1,NM                                                           TRAN 147
       DO 27 J=1,NM                                                           TRAN 148
       IF(I-J) 29,28,29                                                       TRAN 149
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   28 SUM=0.0                                                                TRAN 150
      DO 30 K=1,NM                                                           TRAN 151
      IF(K-I) 31,30,31                                                       TRAN 152
   31 SUM=2.0*XS(I)*XS(K)*WMOL(I)*WMOL(K)*((5./3.)/ASTAR(I,K)+WMOL(K)/       TRAN 153
     1 WMOL(I))/(ETA(I,K)*(WMOL(I)+WMOL(K))**2)+SUM                          TRAN 154
   30 CONTINUE                                                               TRAN 155
      G(I,J)=XS(I)**2/ETA(I,I)+SUM                                           TRAN 156
      GO TO 27                                                               TRAN 157
   29 G(I,J)=-2.0*XS(I)*XS(J)*WMOL(I)*WMOL(J)*((5./3.)/ASTAR(I,J)-1.0)/      TRAN 158
     1 (ETA(I,J)*(WMOL(I)+WMOL(J))**2)                                       TRAN 159
      G(J,I)=G(I,J)                                                          TRAN 160
   27 CONTINUE                                                               TRAN 161
      K=NM+1                                                                 TRAN 162
      DO 32 I=1,NM                                                           TRAN 163
   32 G(I,K)=XS(I)                                                           TRAN 164
      IMAT=NM                                                                TRAN 165
      DO 33 I=1,NM                                                           TRAN 166
      DO 33 J=1,K                                                            TRAN 167
   33 GMAT(I,J)=G(I,J)                                                       TRAN 168
      CALL GAUSS                                                             TRAN 169
      DO 34 I=1,NM                                                           TRAN 170
      CHECK(I)=0.0                                                           TRAN 171
      DO 35 J=1,NM                                                           TRAN 172
   35 CHECK(I)=CHECK(I)+X(J)*GMAT(I,J)                                       TRAN 173
      IF(ABS((CHECK(I)-XS(I))/XS(I))-0.0001) 34,36,36                        TRAN 174
   36 WRITE(6,37) NM,I,CHECK(I),XS(I)                                        TRAN 175
   37 FORMAT(1H1,31X,48HERROR IN GAUSS SOLUTION IN CALCULATING VISCOSITYTRAN 176
     1//3X,10HTHERE ARE  I2,45H EQUATIONS AND THERE IS AN ERROR IN EQUATTRAN 177
     2ICN  I2,26H THE CALCULATED ANSWER IS  F10.7,12H INSTEAD OF  F10.7 TRAN 178
     3//50X,19HTHE MATRIX ARRAY IS/)                                         TRAN 179
      WRITE(6,MATRX)                                                         TRAN 180
   34 CONTINUE                                                               TRAN 181
      DO 39 I=1,NM                                                           TRAN 182
   39 VISC=VISC+XS(I)*X(I)                                                   TRAN 183
C                                                                            TRAN 184
      DO 40 I=1,NM                                                           TRAN 185
      DO 40 J=I,NM                                                           TRAN 186
      IF(I-J) 42,41,42                                                       TRAN 187
   41 SUM=0.0                                                                TRAN 188
      DO 43 K=1,NM                                                           TRAN 189
      IF(K-I) 44,43,44                                                       TRAN 190
   44 SUM=16.0*XS(I)*XS(K)*(7.5*WMOL(I)**2+6.25*WMOL(K)**2-3.0*              TRAN 191
     1 WMOL(K)**2*BSTAR(I,K)+4.0*WMOL(I)*WMOL(K)*ASTAR(I,K))*WMOL(I)*        TRAN 192
     2 WMOL(K)/(15.0*R*(WMOL(I)+WMOL(K))**3*ASTAR(I,K)*ETA(I,K))+SUM         TRAN 193
   43 CONTINUE                                                               TRAN 194
      G(I,J)=16.0*XS(I)**2*WMOL(I)/(15.0*R*ETA(I,I))+SUM                     TRAN 195
      GO TO 40                                                               TRAN 196
   42 G(I,J)=-16.0*XS(I)*XS(J)*WMOL(I)**2*WMOL(J)**2*(13.75-3.0*             TRAN 197
     1 BSTAR(I,J)-4.0*ASTAR(I,J))/(15.0*R*(WMOL(I)+WMOL(J))**3              TRAN 198
     2 *ASTAR(I,J)*ETA(I,J))                                                 TRAN 199
      G(J,I)=G(I,J)                                                          TRAN 200
   40 CONTINUE                                                               TRAN 201
      K=NM+1                                                                 TRAN 202
      DO 45 I=1,NM                                                           TRAN 203
   45 G(I,K)=XS(I)                                                           TRAN 204
      CALL GAUSS                                                             TRAN 205
      DO 47 I=1,NM                                                           TRAN 206
   47 MONCON=MONCON+4.0*XS(I)*X(I)                                           TRAN 207
C                                                                            TRAN 208
C     CALCULATE INTERNAL THERMAL CONDUCTIVITY                                TRAN 209
C                                                                            TRAN 210
      DO 104 I=1,NM                                                          TRAN 211
      IF(CVIBR(I).EQ.0.0) CVIBR(I) = CPRR(I)-(2.5+0.5*ROTM(I))               TRAN 212
      RELXTN(I)=0.0                                                          TRAN 213
      IF(ZROT(I).NE.0.) RELXTN(I)=0.5*ROTM(I)/ZROT(I)                        TRAN 214
      IF(ZVIB(I).NE.0.) RELXTN(I)=RELXTN(I)+CVIBR(I)/ZVIB(I)                 TRAN 215
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  104 CONTINUE                                                          TRAN 216
      DO 53 I=1,NM                                                      TRAN 217
      IF(CPRR(I).EQ.2.5) GO TO 53                                       TRAN 218
      SUM=0.0                                                           TRAN 219
      DO 54 K=1,NM                                                      TRAN 220
      IF(K-I) 55,54,55                                                  TRAN 221
   55 SUM=SUM+ASTAR(I,I)*ETA(I,I)*XS(K)*2.0*WMOL(K)/(ASTAR(I,K)*        TRAN 222
     1 ETA(I,K)*XS(I)*(WMOL(I)+WMOL(K)))                                TRAN 223
   54 CONTINUE                                                          TRAN 224
      INTCON=INTCON+(1.2*ASTAR(I,I)*(CPRR(I)-2.5)-RELXTN(I)*            TRAN 225
     1 (2.5-1.2*ASTAR(I,I))**2/(0.5*PI+RELXTN(I)*(5.0/3.0+1.2*          TRAN 226
     2 ASTAR(I,I)/(CPRR(I)-2.5))))*R*ETA(I,I)/WMOL(I)/(1.0+SUM)         TRAN 227
   53 CONTINUE                                                          TRAN 228
      IF(NR.EQ.0) GO TO 91                                              TRAN 229
      IF(FROZN) GO TO 91                                                TRAN 230
C                                                                       TRAN 231
C     CALCULATE REACTION HEAT CAPACITY AND THERMAL CONDUCTIVITY         TRAN 232
C                                                                       TRAN 233
      L=1+NR                                                            TRAN 234
      SUM1=0.0                                                          TRAN 235
      SUM2=0.0                                                          TRAN 236
      DO 65 I=1,NR                                                      TRAN 237
      DELH(I)=0.0                                                       TRAN 238
      DO 66 K=1,NM                                                      TRAN 239
   66 DELH(I)=STC(I,K)*HRRT(K)+DELH(I)                                  TRAN 240
   65 G(I,L)=DELH(I)                                                    TRAN 241
      JJ=NM-1                                                           TRAN 242
      DO 99 K=1,JJ                                                      TRAN 243
      LL=K+1                                                            TRAN 244
      DO 99 L=LL,NM                                                     TRAN 245
      RTPD(K,L)= WMOL(K)*WMOL(L)/                                       TRAN 246
     1 (ASTAR(K,L)*ETA(K,L)*(WMOL(K)+WMOL(L)))                          TRAN 247
      XSKL(K,L) = 1.0/(XS(K)*XS(L))                                     TRAN 248
      XSKL(L,K) = XSKL(K,L)                                             TRAN 249
   99 RTPD(L,K) = RTPD(K,L)                                             TRAN 250
      DO 98 I=1,17                                                      TRAN 251
      DO 98 J=1,20                                                      TRAN 252
   98 IF (ABS(STC(I,J)).LT.1.0E-6)  STC(I,J) = 0.0                      TRAN 253
      DO 67 I=1,NR                                                      TRAN 254
      DO 67 J=I,NR                                                      TRAN 255
      DO 68 K=1,JJ                                                      TRAN 256
      LL=K+1                                                            TRAN 257
      DO 68 L=LL,NM                                                     TRAN 258
      STXS(K,L) = 0.0                                                   TRAN 259
      IF ((STC(I,K).EQ.0.0).AND.(STC(I,L).EQ.0.0))  GO TO 68            TRAN 260
      IF ((STC(J,K).EQ.0.0).AND.(STC(J,L).EQ.0.0))  GO TO 68            TRAN 261
      STXS(K,L) = XSKL(K,L)*                                            TRAN 262
     1 (XS(L)*STC(I,K)-XS(K)*STC(I,L))*                                 TRAN 263
     2 (XS(L)*STC(J,K)-XS(K)*STC(J,L))                                  TRAN 264
      SUM1 = SUM1+STXS(K,L)                                             TRAN 265
      SUM2 = SUM2+RTPD(K,L)*STXS(K,L)                                   TRAN 266
   68 CONTINUE                                                          TRAN 267
      GMAT(I,J) = SUM2                                                  TRAN 268
      SUM2=0.0                                                          TRAN 269
      GMAT(J,I) = GMAT(I,J)                                             TRAN 270
      G(I,J) = SUM1                                                     TRAN 271
      SUM1=0.0                                                          TRAN 272
   67 G(J,I)=G(I,J)                                                     TRAN 273
      IMAT=NR                                                           TRAN 274
      CALL GAUSS                                                        TRAN 275
      DO 101 I=1,NR                                                     TRAN 276
  101 CPREAC=CPREAC+R*DELH(I)*X(I)                                      TRAN 277
C                                                                       TRAN 278
      L=1+NR                                                            TRAN 279
      DO 57 I=1,NR                                                      TRAN 280
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   57 G(I,L)=DELH(I)                                                    TRAN 281
      JJ=NM-1                                                           TRAN 282
      DO 59 I=1,NR                                                      TRAN 283
      DO 59 J=I,NR                                                      TRAN 284
      G(I,J) = GMAT(I,J)                                                TRAN 285
   59 G(J,I)=G(I,J)                                                     TRAN 286
      CALL GAUSS                                                        TRAN 287
      DO 70 I=1,NR                                                      TRAN 288
      CHECK(I)=0.0                                                      TRAN 289
      DO 71 J=1,NR                                                      TRAN 290
   71 CHECK(I)=CHECK(I)+X(J)*GMAT(I,J)                                  TRAN 291
      IF(ABS((CHECK(I)-DELH(I))/DELH(I))-0.010) 70,72,72                TRAN 292
   72 WRITE(6,73) NR,I,CHECK(I),DELH(I)                                 TRAN 293
   73 FORMAT(1H1,31X,68HERROR IN GAUSS SOLUTION IN CALCULATING REACTION TRAN 294
     1THERMAL CONDUCTIVITY//3X,10HTHERE ARE I2,45H EQUATIONS AND THERE ITRAN 295
     2S AN ERROR IN EQUATION I2,26H THE CALCULATED ANSWER IS F10.7,     TRAN 296
     312H INSTEAD OF F10.7//50X,19HTHE MATRIX ARRAY IS/)                TRAN 297
      WRITE(6,MATRX)                                                    TRAN 298
   70 CONTINUE                                                          TRAN 299
      DO 75 I=1,NR                                                      TRAN 300
   75 REACON=REACON+R*DELH(I)*X(I)                                      TRAN 301
      REACON = (3./5.)*REACON                                           TRAN 302
C                                                                       TRAN 303
C     CALCULATE OTHER ANSWERS                                           TRAN 304
C                                                                       TRAN 305
   91 FRZCON=MONCON+INTCON                                              TRAN 306
      EQCON=FRZCON+REACON                                               TRAN 307
      DO 102 I=1,NM                                                     TRAN 308
      CPFROZ=CPFROZ+XS(I)*CPRR(I)                                       TRAN 309
      ENTLPY=ENTLPY+XS(I)*HRRT(I)                                       TRAN 310
  102 WTMOL=WTMOL+XS(I)*WMOL(I)                                         TRAN 311
      CPFROZ=CPFROZ*R/WTMOL                                             TRAN 312
      CPREAC=CPREAC/WTMOL                                               TRAN 313
      CPEQ=CPREAC+CPFROZ                                                TRAN 314
      ENTLPY=R*TT*ENTLPY/WTMOL                                          TRAN 315
      PRFROZ=VISC*CPFROZ/FRZCON                                         TRAN 316
      PREQ=VISC*CPEQ/EQCON                                              TRAN 317
      PREQ=VISC*CPEQ/EQCON                                              TRAN 318
      DENSTY=(WTMOL*PP)/(RPVT*TT)                                       TRAN 319
      IF(FROZN.OR.NR.EQ.0) GO TO 105                                    TRAN 320
      LEWIS=(REACON*CPFROZ)/(FRZCON*CPREAC)                             TRAN 321
  105 CONTINUE                                                          TRAN 322
C                                                                       TRAN 323
      CALL OUT                                                          TRAN 324
C                                                                       TRAN 325
    3 CONTINUE                                                          TRAN 326
      RETURN                                                            TRAN 327
      END                                                               TRAN 328
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C
      SUBROUTINE INPUT                                                  INPT   1
C                                                                       INPT   2
C     BRINGS IN AND SORTS OUT INPUT FOR TRANSPORT CALCULATIONS          INPT   3
C                                                                       INPT   4
      DOUBLE PRECISION G,X                                              INPT   5
      INTEGER SUB,SPECIE,SPECE                                          INPT   6
      REAL MONCON,INTCON,LEWIS                                          INPT   7
      LOGICAL TRNSPT,FROZN,PUNCH,NODATA                                 INPT   8
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C                                                                       INPT   9
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     INPT  10
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  INPT  11
     2 VLM(13),TOTN(13)                                                 INPT  12
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), INPT  13
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   INPT  14
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),INPT  15
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      INPT  16
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         INPT  17
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FCX(15),DENS(15),INPT  18
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      INPT  19
      COMMON /DOUBLE/ G(20,21), X(20)                                   INPT  20
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   INPT  21
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, INPT  22
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JSI,VOL,IT,CALCH,NLS,LOGV, INPT  23
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            INPT  24
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),        INPT  25
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       INPT  26
     2 APPL,ARATIO,ELN                                                  INPT  27
      COMMON /SAVED/SLN(10C),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,    INPT  28
     1 LLL,LM,MAXNP,STORE(52,16),XS(20),WMOL(20),IND(20),NM,            INPT  29
     2 FIRSTP,FIRSTV                                                    INPT  30
      COMMON /TRANS/ TEM(100,20),TABLES(100,20,3),SPECIE(100,2,3),      INPT  31
     1 OMEGA(20,20),ASTAR(20,20),BSTAR(20,20),CPRR(20),                 INPT  32
     2 HRRT(20),ZROT(20),ZVIB(20),CVIBR(20),ROTM(20),RELXTN(20),        INPT  33
     3 ROTNM(80),STCF(17,20),STC(17,20),STCOEF(20),ANS(15),             INPT  34
     4 SPECE(2,3),NTT(100),NTAB(100),NR,N                               INPT  35
      COMMON /INTERP/ Z(20),Y(20,3),NTP,ANSR(3)                         INPT  36
      COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA                          INPT  37
C                                                                       INPT  38
      DIMENSION IATOM(3,101)                                            INPT  39
C                                                                       INPT  40
      EQUIVALENCE (ATOM,IATOM)                                          INPT  41
      EQUIVALENCE (ANS(1) ,VISC  ), (ANS(2) ,MONCON), (ANS(3) ,INTCON)  INPT  42
      EQUIVALENCE (ANS(4) ,FRZCON), (ANS(5) ,REACON), (ANS(6) ,EQCON )  INPT  43
      EQUIVALENCE (ANS(7) ,CPFROZ), (ANS(8) ,CPEQ  ), (ANS(9) ,PRFROZ)  INPT  44
      EQUIVALENCE (ANS(10),PREQ  ), (ANS(11),LEWIS ), (ANS(12),WTMOL )  INPT  45
      EQUIVALENCE (ANS(13),DENSTY), (ANS(14),CPREAC), (ANS(15),ENTLPY)  INPT  46
C                                                                       INPT  47
      DATA MAXNM/20/,ND/4HLAST/,NBLANK/1H /                             INPT  48
C                                                                       INPT  49
C                                                                       INPT  50
C     PICK OUT ELEMENTS                                                 INPT  51
C                                                                       INPT  52
      IF(FROZN.AND.N.GT.NFZ) GO TO 92                                   INPT  53
      IF(FROZN.AND.MAXNP.GT.12) GO TO 92                                INPT  54
      NSP=NS                                                            INPT  55
      DO 1 J=1,NLM                                                      INPT  56
      DO 2 I=1,NS                                                       INPT  57
      IF(LLMT(J).NE.SUB(I,1)) GO TO 2                                   INPT  58
      SUMA=0.0                                                          INPT  59
      DO 60 K=1,NLM                                                     INPT  60
   60 SUMA=SUMA+A(K,I)                                                  INPT  61
      IF(SUMA.NE.1.) GO TO 2                                            INPT  62
      IND(J)=I                                                          INPT  63
      GO TO 1                                                           INPT  64
    2 CONTINUE                                                          INPT  65
      WRITE(6,61) LLMT(J)                                               INPT  66
   61 FORMAT(1HO,15X,58HNO ELEMENT WAS FOUND IN THE LIST OF SPECIES WITHINPT  67
     1 THE NAME A3,45HOR ELSE THERE IS AN ERROR IN THE A(I,K) ARRAY)    INPT  68
      NSP=NSP+1                                                         INPT  69
      IND(J) = NSP                                                      INPT  70
      EN(NSP,N) = 0.0                                                   INPT  71
      DO 3 K=1,NLM                                                      INPT  72
    3 A(K,NSP) = 0.0                                                    INPT  73
      A(J,NSP) = 1.0                                                    INPT  74
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      SUB(NSP,1) = LLMT(J)                                              INPT  75
      SUB(NSP,2) = NBLANK                                               INPT  76
      SUB(NSP,3) = NBLANK                                               INPT  77
    1 CONTINUE                                                          INPT  78
C                                                                       INPT  79
C     PICK OUT IMPORTANT SPECIES                                        INPT  80
C                                                                       INPT  81
      NM=NLM                                                            INPT  82
      DO 4 I=1,NLM                                                      INPT  83
      J=IND(I)                                                          INPT  84
      EN(J,N)=-EN(J,N)                                                  INPT  85
    4 CONTINUE                                                          INPT  86
      TESTEN=(1.E-7)/WM(N)                                              INPT  87
    5 BIGEN=(1.E-7)/WM(N)                                               INPT  88
      DO 6 J=1,NSP                                                      INPT  89
      IF(IUSE(J).NE.0) GO TO 6                                          INPT  90
      IF(EN(J,N).LT.BIGEN) GO TO 6                                      INPT  91
      BIGEN=EN(J,N)                                                     INPT  92
    6 CONTINUE                                                          INPT  93
      IF(BIGEN.EQ.TESTEN) GO TO 7                                       INPT  94
      DO 59 J=1,NSP                                                     INPT  95
      IF (BIGEN.NE.EN(J,N)) GO TO 59                                    INPT  96
      EN(J,N)=-EN(J,N)                                                  INPT  97
      NM=NM+1                                                           INPT  98
      IND(NM)=J                                                         INPT  99
   59 CONTINUE                                                          INPT 100
      IF(NM.LT.MAXNM) GO TO 5                                           INPT 101
    7 DO 8 I=1,NM                                                       INPT 102
      J=IND(I)                                                          INPT 103
      EN(J,N)=-EN(J,N)                                                  INPT 104
    8 CONTINUE                                                          INPT 105
C                                                                       INPT 106
C     CALCULATE MOLE FRACTIONS FROM THE EN(J,N)                         INPT 107
C                                                                       INPT 108
      TOTAL=0.0                                                         INPT 109
      DO 10 I=1,NM                                                      INPT 110
      J=IND(I)                                                          INPT 111
      XS(I)=EN(J,N)                                                     INPT 112
      TOTAL=EN(J,N)+TOTAL                                               INPT 113
   10 CONTINUE                                                          INPT 114
      DO 11 I=1,NM                                                      INPT 115
   11 XS(I)=XS(I)/TOTAL                                                 INPT 116
      DO 31 I=1,NM                                                      INPT 117
   31 IF(XS(I).LT.1.E-10) XS(I)=1.E-10                                  INPT 118
C                                                                       INPT 119
C     CALCULATE MOLECULAR WEIGHTS                                       INPT 120
C                                                                       INPT 121
      DO 12 I=1,NM                                                      INPT 122
      WMOL(I)=0.0                                                       INPT 123
   12 CONTINUE                                                          INPT 124
      DO 32 I=1,NLM                                                     INPT 125
      DO 33 K=1,101                                                     INPT 126
      IF(LLMT(I).EQ.IATOM(1,K)) GO TO 34                                INPT 127
   33 CONTINUE                                                          INPT 128
   34 DO 35 J=1,NM                                                      INPT 129
      L=IND(J)                                                          INPT 130
      WMOL(J)=WMOL(J)+ATOM(2,K)*A(I,L)                                  INPT 131
   35 CONTINUE                                                          INPT 132
   32 CONTINUE                                                          INPT 133
   92 CONTINUE                                                          INPT 134
C                                                                       INPT 135
C     FIND TRANSPORT AND RELAXATON DATA FOR IMPORTANT INTERACTIONS      INPT 136
C                                                                       INPT 137
      DO 9 I=1,NM                                                       INPT 138
      ZROT(I) = 0.0                                                     INPT 139
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      ROTM(I) = 0.0                                                     INPT 140
      ZVIB(I) = 0.0                                                     INPT 141
      CVIBR(I) = 0.0                                                    INPT 142
      DO 9 J=1,NM                                                       INPT 143
      OMEGA(I,J)=0.0                                                    INPT 144
    9 CONTINUE                                                          INPT 145
      NK=0                                                              INPT 146
   18 NK=NK+1                                                           INPT 147
      IF(SPECIE(NK,1,1).EQ.ND) GO TO 22                                 INPT 148
      K=1                                                               INPT 149
   14 DO 16 L=1,NM                                                      INPT 150
      J=IND(L)                                                          INPT 151
      DO 15 I=1,3                                                       INPT 152
      IF(SPECIE(NK,K,I).NE.SUB(J,I)) GO TO 16                           INPT 153
   15 CONTINUE                                                          INPT 154
      IF(K.EQ.2) GO TO 20                                               INPT 155
      M=L                                                               INPT 156
      GO TO 17                                                          INPT 157
   16 CONTINUE                                                          INPT 158
      GO TO 18                                                          INPT 159
   17 JJ=J                                                              INPT 160
      DO 19 I=1,3                                                       INPT 161
      IF(SPECIE(NK,2,I).NE.SUB(J,I)) GO TO 24                           INPT 162
   19 CONTINUE                                                          INPT 163
      GO TO 20                                                          INPT 164
   24 K=2                                                               INPT 165
      GO TO 14                                                          INPT 166
   20 NTP=NTT(NK)                                                       INPT 167
      DO 39 I=1,NTP                                                     INPT 168
      T(I)=TEM(NK,I)                                                    INPT 169
      DO 39 J=1,3                                                       INPT 170
      Y(I,J)=TABLES(NK,I,J)                                             INPT 171
   39 CONTINUE                                                          INPT 172
      CALL LGRNGE(TT)                                                   INPT 173
      IF(NTAB(NK).EQ.1) GO TO 21                                        INPT 174
      ROTM(M)=ROTNM(NK)                                                 INPT 175
      ZROT(M)=ANSR(1)                                                   INPT 176
      ZVIB(M)=ANSR(2)                                                   INPT 177
      CVIBR(M)=ANSR(3)                                                  INPT 178
      GO TO 18                                                          INPT 179
   21 CONTINUE                                                          INPT 180
      OMEGA(L,M)=ANSR(1)                                                INPT 181
      ASTAR(L,M)=ANSR(2)                                                INPT 182
      BSTAR(L,M)=ANSR(3)                                                INPT 183
      IF(J.EQ.JJ) GO TO 18                                              INPT 184
      OMEGA(M,L)=OMEGA(L,M)                                             INPT 185
      ASTAR(M,L)=ASTAR(L,M)                                             INPT 186
      BSTAR(M,L)=BSTAR(L,M)                                             INPT 187
      GO TO 18                                                          INPT 188
C                                                                       INPT 189
C     MAKE ESTIMATES FOR MISSING DATA                                   INPT 190
C                                                                       INPT 191
   22 DO 27 I=1,NM                                                      INPT 192
      IF(OMEGA(I,I).NE.0.) GO TO 27                                     INPT 193
      K=IND(I)                                                          INPT 194
      IF(XS(I).LT.5.0E-6) GO TO 36                                      INPT 195
      IF(NODATA) GO TO 36                                               INPT 196
      WRITE(6,28) (SUB(K,L),L=1,3)                                      INPT 197
   28 FORMAT(1HO,40X,45HNO TRANSPORT DATA WERE FOUND FOR THE SPECIES 3A4INPT 198
     1)                                                                 INPT 199
   36 CONTINUE                                                          INPT 200
      OMEGA(I,I) = ALOG (320.*WMOL(I)**4/TT**1.4)                       INPT 201
      IF (OMEGA(I,I).LT.1.) OMEGA(I,I) = 1.                             INPT 202
      ASTAR(I,I)=1.0                                                    INPT 203
      BSTAR(I,I)=1.0                                                    INPT 204
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   27 CONTINUE                                                                    INPT 205
      NMM=NM-1                                                                    INPT 206
      DO 23 I=1,NMM                                                               INPT 207
      K=I+1                                                                       INPT 208
      DO 23 J=K,NM                                                                INPT 209
      IF(OMEGA(I,J).NE.0.) GO TO 26                                               INPT 210
      OMEGA(I,J)=(OMEGA(I,I)+OMEGA(J,J)+2.*SQRT(OMEGA(I,I)*OMEGA(J,J)))           INPT 211
     1/4.0                                                                        INPT 212
      ASTAR(I,J)=(ASTAR(I,I)+ASTAR(J,J))/2.                                       INPT 213
      BSTAR(I,J)=(BSTAR(I,I)+BSTAR(J,J))/2.                                       INPT 214
   26 OMEGA(J,I)=OMEGA(I,J)                                                       INPT 215
      ASTAR(J,I)=ASTAR(I,J)                                                       INPT 216
      BSTAR(J,I)=BSTAR(I,J)                                                       INPT 217
   23 CONTINUE                                                                    INPT 218
      IF(FROZN) GO TO 96                                                          INPT 219
C                                                                                 INPT 220
C     REWRITE REACTIONS TO ELIMINATE TRACE SPECIES                                INPT 221
C                                                                                 INPT 222
      LL=NLM+1                                                                    INPT 223
      NR=NM-NLM                                                                   INPT 224
      IF(NR.EQ.0) GO TO 96                                                        INPT 225
      DO 30 K=1,17                                                                INPT 226
      DO 30 L=1,20                                                                INPT 227
   30 STC(K,L)=0.0                                                                INPT 228
      K=1                                                                         INPT 229
      DO 62 I=LL,NM                                                               INPT 230
      STC(K,I)=-1.0                                                               INPT 231
      J=IND(I)                                                                    INPT 232
      DO 63 L=1,NLM                                                               INPT 233
   63 STC(K,L)=A(L,J)                                                             INPT 234
      K=K+1                                                                       INPT 235
   62 CONTINUE                                                                    INPT 236
      I=1                                                                         INPT 237
      NN=I                                                                        INPT 238
   81 IF(XS(I).LT.1.0E-07) GO TO 97                                               INPT 239
   98 I=I+1                                                                       INPT 240
      NN=I                                                                        INPT 241
      IF(I-NM) 81,81,96                                                           INPT 242
   97 L=1                                                                         INPT 243
      J=1                                                                         INPT 244
   80 IF(ABS(STC(J,I)).GT.1.0E-06)  GO TO 95                                      INPT 245
      DO 79 K=1,NM                                                                INPT 246
   79 STCF(L,K)=STC(J,K)                                                          INPT 247
      L=L+1                                                                       INPT 248
      IF(J.GE.NR) GO TO 98                                                        INPT 249
      J=J+1                                                                       INPT 250
      GO TO 80                                                                    INPT 251
   95 COEFF=STC(J,I)                                                              INPT 252
      DO 90 K=1,NM                                                                INPT 253
   90 STCOEF(K)=STC(J,K)/COEFF                                                    INPT 254
      GO TO 77                                                                    INPT 255
   84 J=J+1                                                                       INPT 256
      IF(ABS(STC(J,I)).LT.1.0E-06)  GO TO 89                                      INPT 257
      COEFF=STC(J,I)                                                              INPT 258
      DO 87 K=1,NM                                                                INPT 259
   87 STC(J,K)=(STC(J,K)/COEFF)-STCOEF(K)                                         INPT 260
   89 DO 85 K=1,NM                                                                INPT 261
   85 STCF(L,K)=STC(J,K)                                                          INPT 262
      L=L+1                                                                       INPT 263
   77 IF(J.LT.NR) GO TO 84                                                        INPT 264
      DO 82 I=1,NM                                                                INPT 265
      DO 82 J=1,NR                                                                INPT 266
   82 STC(J,I)=STCF(J,I)                                                          INPT 267
      I=NN                                                                        INPT 268
      NR=L-1                                                                      INPT 269
      GO TO 98                                                                    INPT 270
```

```
   96 CONTINUE                                                          INPT 271
      RETURN                                                            INPT 272
      END                                                               INPT 273


C
      SUBROUTINE OUT                                                    OUT    1
C                                                                       OUT    2
C     SETS UP AND WRITES OUTPUT FOR TRANSPORT PROPERTIES                OUT    3
C                                                                       OUT    4
      DOUBLE PRECISION G,X                                              OUT    5
      INTEGER SUB,SPECIE,SPECE                                          OUT    6
      REAL MONCON,INTCON,LEWIS,INTRNL                                   OUT    7
      LOGICAL TRNSPT,FROZN,PUNCH,NODATA                                 OUT    8
      LOGICAL TP,HP,SP,DETN,SHOCK,RKT,EQL,VOL                           OUT    9
C                                                                       OUT   10
      COMMON /POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13),     OUT   11
     1 GAMMAS(13),P(26),T(52),V(13),PPP(13),WM(13),SONVEL(13),TTT(13),  OUT   12
     2 VLM(13),TOTN(13)                                                 OUT   13
      COMMON /SPECES/COEF(2,7,100),S(100),HO(100),DELN(100),DUMMY(100), OUT   14
     1 EN(100,13),ENLN(100),A(10,100),SUB(100,3),IUSE(100),TEMP(50,2)   OUT   15
      COMMON /MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(10),BO(10),BOP(10,2),OUT   16
     1 TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBO,AM(2),      OUT   17
     2 HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5),         OUT   18
     3 ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15),OUT   19
     4 RHOP,RMW(15),TLN,CR,OXF(15),ENNL,TRACE,LLMTS(10),SBOP(10,2)      OUT   20
      COMMON /DOUBLE/ G(20,21), X(20)                                   OUT   21
      COMMON /INDX/IDEBUG,CONVG,TP,HP,SP,ISV,NPP,MOLES,NP,NT,NPT,NLM,   OUT   22
     1 NS,KMAT,IMAT,IQ1,IOF,NOF,NOMIT,IP,NEWR,NSUB,NSUP,RKT,DETN,SHOCK, OUT   23
     2 IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,IT,CALCH,NLS,LOGV, OUT   24
     3 ISUP,ISUB,ITNUM,ITM,INCDFZ,INCDEQ,CPRF,IPP,SEQL,PCPLT            OUT   25
      COMMON /PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUPAR(13),        OUT   26
     1 SUPAR(13),APP(13),AEAT(13),CSTR,EQL,FROZ,SSO,AREA,AWT,NFZ,       OUT   27
     2 APPL,ARATIO,ELN                                                  OUT   28
      COMMON /SAVED/SLN(100),IQSAVE,ENSAVE,ENLSAV,LSAVE,JSOLS,JLIQS,    OUT   29
     1 LLL,LM,MAXNP,STORE(52,16),XSI(20),WMOL(20),IND(20),NM,           OUT   30
     2 FIRSTP,FIRSTV                                                    OUT   31
      COMMON /TRANS/ TEM(100,20),TABLES(100,20,3),SPECIE(100,2,3),      OUT   32
     1 OMEGA(20,20),ASTAR(20,20),BSTAR(20,20),CPRR(20),                 OUT   33
     2 HRRT(20),ZROT(20),ZVIB(20),CVIBR(20),ROTM(20),RELXTN(20),        OUT   34
     3 ROTNM(80),STCF(17,20),STC(17,20),STCOEF(20),ANS(15),             OUT   35
     4 SPECE(2,3),NTT(100),NTAB(100),NR,N                               OUT   36
      COMMON /INTERP/ Z(20),Y(20,3),NTP,ANSR(3)                         OUT   37
      COMMON /CONTRL/TRNSPT,FROZN,PUNCH,NODATA                          OUT   38
C                                                                       OUT   39
      EQUIVALENCE (ANS(1) ,VISC  ), (ANS(2) ,MONCON), (ANS(3) ,INTCON)  OUT   40
      EQUIVALENCE (ANS(4) ,FRZCON), (ANS(5) ,REACON), (ANS(6) ,EQCON )  OUT   41
      EQUIVALENCE (ANS(7) ,CPFROZ), (ANS(8) ,CPEQ  ), (ANS(9) ,PRFROZ)  OUT   42
      EQUIVALENCE (ANS(10),PREQ  ), (ANS(11),LEWIS ), (ANS(12),WTMOL )  OUT   43
      EQUIVALENCE (ANS(13),DENSTY), (ANS(14),CPREAC), (ANS(15),ENTLPY)  OUT   44
C                                                                       OUT   45
      ENTLPY = HSUBO*R                                                  OUT   46
      ENTRPY = SO*R                                                     OUT   47
      FPC = 100./(1.+OF)                                                OUT   48
      IF(N.NE.1) GO TO 134                                              OUT   49
      IF(ISV.EQ.0.AND.MAXNP.GT.12) GO TO 134                            OUT   50
      IF(MAXNP.GT.51.OR.(LM.GT.52.AND.LM.LT.66)) GO TO 134              OUT   51
      LM=1                                                              OUT   52
      IF(MAXNP.LT.1) MAXNP=0                                            OUT   53
                                                                        OUT   54
```

```
  134 CONTINUE                                                          OUT   55
      ITT= TT + 0.5                                                     OUT   56
      IF(MAXNP.GT.51.OR.LM.GT.52) GO TO 127                             OUT   57
      IF(ISV.NE.0) GO TO 123                                            OUT   58
      IF(MAXNP.GT.12) GO TO 127                                         OUT   59
      GO TO 124                                                         OUT   60
C                                                                       OUT   61
C     STORE DATA                                                        OUT   62
C                                                                       OUT   63
  123 IF(MAXNP.EQ.0) FIRSTP = PP                                        OUT   64
      IF(MAXNP.EQ.0) FIRSTV = VLM(1)                                    OUT   65
      STORE(MAXNP+1,1)=TT                                               OUT   66
      DO 128 J=1,15                                                     OUT   67
  128 STORE(MAXNP+1,J+1)=ANS(J)                                         OUT   68
      MAXNP=MAXNP+1                                                     OUT   69
      GO TO 132                                                         OUT   70
  127 IF(LM.GT.MAXNP) MAXNP=0                                           OUT   71
      IF(LM.GT.MAXNP) GO TO 104                                         OUT   72
  129 LM=1                                                              OUT   73
  132 IF(LM.GT.MAXNP) GO TO 137                                         OUT   74
      ITT=STORE(LM,1)+0.5                                               OUT   75
      TT=STORE(LM,1)                                                    OUT   76
      DO 131 K=1,15                                                     OUT   77
  131 ANS(K)=STORE(LM,K+1)                                              OUT   78
      IF(LM.GT.1) GO TO 104                                             OUT   79
  124 IF(N.NE.1) GO TO 104                                              OUT   80
      IF(ISV.EQ.0.AND.LM.NE.1) GO TO 104                                OUT   81
C                                                                       OUT   82
C     WRITE HEADING FOR DATA                                            OUT   83
C                                                                       OUT   84
      WRITE(6,1)                                                        OUT   85
    1 FORMAT(1H1)                                                       OUT   86
      IF(MAXNP.LT.13) FIRSTP = PP                                       OUT   87
      IF(MAXNP.LT.13) FIRSTV = VLM(1)                                   OUT   88
      IF(DETN) GO TO 6                                                  OUT   89
      IF(SHOCK) GO TO 7                                                 OUT   90
      IF(RKT) GO TO 8                                                   OUT   91
      IF(VOL) GO TO 3                                                   OUT   92
      IF(TP) GO TO 2                                                    OUT   93
      IF(HP) GO TO 4                                                    OUT   94
      IF(SP) GO TO 5                                                    OUT   95
    3 IF(TP) WRITE(6,16)                                                OUT   96
   16 FORMAT(1HO,38X,55HTRANSPORT PROPERTIES AT ASSIGNED TEMPERATURE ANDOUT   97
     1 VOLUME/)                                                         OUT   98
      IF(TP) WRITE(6,20) OF,FPC,EQRAT,FIRSTV                            OUT   99
   20 FORMAT (1HO,12X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,        OUT  100
     1  19HEQUIVALENCE RATIO= ,F7.4,4X,13HFIRST VOLUME=F8.2,            OUT  101
     2  1X,4HCC/G///)                                                  OUT  102
      IF(TP) GO TO 155                                                  OUT  103
      IF(SP) WRITE(6,17)                                                OUT  104
   17 FORMAT(1HO,41X,51HTRANSPORT PROPERTIES AT ASSIGNED ENTROPY AND VOLOUT  105
     1UME/)                                                             OUT  106
      IF(SP) GO TO 14                                                   OUT  107
      WRITE(6,141)                                                      OUT  108
  141 FORMAT(1HO,46X,39HTRANSPORT PROPERTIES AT ASSIGNED VOLUME/)       OUT  109
      INTRNL = ENTLPY                                                   OUT  110
      WRITE(6,15) OF,FPC,EQRAT,INTRNL                                   OUT  111
   15 FORMAT (1HO,11X,4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,         OUT  112
     1  19HEQUIVALENCE RATIO= ,F7.4,4X,16HINTERNAL ENERGY=F8.2,         OUT  113
     2  6H CAL/G ///)                                                  OUT  114
      GO TO 155                                                         OUT  115
    2 WRITE(6,140)                                                      OUT  116
  140 FORMAT(1HO,37X,57HTRANSPORT PROPERTIES AT ASSIGNED TEMPERATURE ANDOUT  117
     1 PRESSURE/)                                                       OUT  118
   13 WRITE(6,147) OF,FPC,EQRAT,FIRSTP                                  OUT  119
```

```
147 FORMAT (1HO,12X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,          OUT  120
   1  19HEQUIVALENCE RATIO= ,F7.4,4X,15HFIRST PRESSURE=F8.3,           OUT  121
   2  1X,3HATM///)                                                     OUT  122
     GO TO 155                                                        OUT  123
   4 WRITE(6,142)                                                     OUT  124
142 FORMAT(1HO,44X,42HTRANSPORT PROPERTIES AT ASSIGNED PRESSURES/)     OUT  125
     WRITE(6,149) OF,FPC,EQRAT,ENTLPY                                 OUT  126
149 FORMAT (1HO,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,         OUT  127
   1  19HEQUIVALENCE RATIO= ,F7.4,4X,9HENTHALPY=F8.1,6H CAL/G///)      OUT  128
     GO TO 155                                                        OUT  129
   5 WRITE(6,143)                                                     OUT  130
143 FORMAT(1HO,39X,53HTRANSPORT PROPERTIES AT ASSIGNED ENTROPY AND PREOUT  131
   1SSURE/)                                                         OUT  132
  14 WRITE(6,150) OF,FPC,EQRAT,ENTRPY                               OUT  133
150 FORMAT (1HO,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,         OUT  134
   1  19HEQUIVALENCE RATIO= ,F7.4,4X,8HENTROPY=F8.4,11H CAL/(G)(K)///)OUT  135
     GO TO 155                                                        OUT  136
   6 WRITE(6,144)                                                     OUT  137
144 FORMAT(1HO,45X,41HTRANSPORT PROPERTIES OF THE DETONATED GAS/)      OUT  138
     WRITE(6,151) OF,FPC,EQRAT,FIRSTP                                 OUT  139
151 FORMAT (1HO,16X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,         OUT  140
   1  19HEQUIVALENCE RATIO= ,F7.4,4X,26HFIRST DETONATION PRESSURE=     OUT  141
   2  F8.3,1X,3HATM///)                                              OUT  142
     GO TO 155                                                        OUT  143
   7 IF (FROZN) GO TO 9                                               OUT  144
     WRITE(6,154)                                                     OUT  145
154 FORMAT(1HO,27X,72HTRANSPORT PROPERTIES OF THE SHOCKED GAS ASSUMINGOUT  146
   1 EQUILIBRIUM COMPOSITION/)                                      OUT  147
     GO TO 10                                                         OUT  148
   9 WRITE(6,157)                                                     OUT  149
157 FORMAT(1HO,27X,67HTRANSPORT PROPERTIES OF THE SHOCKED GAS ASSUMINGOUT  150
   1 FROZEN COMPOSITION/)                                           OUT  151
  10 WRITE(6,152) OF,FPC,EQRAT,PPP(1)                               OUT  152
152 FORMAT (1HO,10X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,         OUT  153
   1  19HEQUIVALENCE RATIO= ,F7.4,4X,21HFIRST SHOCK PRESSURE=F9.4,     OUT  154
   2  1X,3HATM///)                                                   OUT  155
     GO TO 155                                                        OUT  156
   8 IF (FROZN) GO TO 11                                              OUT  157
     WRITE(6,156)                                                     OUT  158
156 FORMAT(1HO,21X,88HTRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING OUT  159
   1EQUILIBRIUM COMPOSITION DURING EXPANSION/)                       OUT  160
     GO TO 12                                                         OUT  161
  11 WRITE(6,158)                                                     OUT  162
158 FORMAT(1HO,24X,83HTRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING OUT  163
   1FROZEN COMPOSITION DURING EXPANSION/)                           OUT  164
     IF(.NOT.EQL.AND.NFZ.NE.1) WRITE(6,159) NFZ                       OUT  165
159 FORMAT(56X,18HFROZEN AFTER POINT, I2  /)                          OUT  166
  12 WRITE(6,153) OF,FPC,EQRAT,PPP(1)                               OUT  167
153 FORMAT (1HO,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,         OUT  168
   1  19HEQUIVALENCE RATIO= ,F7.4,4X,17HCHAMBER PRESSURE=F8.3,         OUT  169
   2  1X,3HATM///)                                                   OUT  170
155 CONTINUE                                                          OUT  171
     IF(.NOT.FROZN) GO TO 105                                         OUT  172
     WRITE(6,106)                                                     OUT  173
106 FORMAT (32X,4HTEMP,3X,9HVISCOSITY,2X,9HMONATOMIC,2X,8HINTERNAL,4X,OUT  174
   16HFROZEN,6X,2HCP,8X,7HPRANDTL/52X,4HCOND,7X,4HCOND,7X,4HCOND,9X,  OUT  175
   24HFROZ,5X,4HFROZ//31X,5HDEG K,5X,5HPOISE,5X,27H----- CAL/(CM)(SEC)OUT  176
   1(K) ----,5X,10HCAL/(G)(K)///)                                   OUT  177
     WRITE(6,107) ITT,(ANS(I),I=1,4),ANS(7),ANS(9)                    OUT  178
107 FORMAT(30X,I6,F9.0,5HX10-6,F6.0,5HX10-6,F6.0,5HX10-6,F6.0,5HX10-6,OUT  179
   1F8.4,F10.4)                                                     OUT  180
     GO TO 108                                                        OUT  181
105 WRITE(6,109)                                                      OUT  182
109 FORMAT (2X,4HTEMP,3X,9HVISCOSITY,2X,9HMONATOMIC,2X,8HINTERNAL,4X, OUT  183
   16HFROZEN,5X,8HREACTION,3X,11HEQUILIBRIUM,3X,2HCP,9X,2HCP,7X,      OUT  184
   27HPRANDTL,3X,7HPRANDTL,4X,5HLEWIS/22X,4HCOND,7X,4HCOND,7X,4HCOND, OUT  185
```

```
     38X,4HCOND,8X,4HCOND,9X,4HFROZ,7X,2HEQ,6X,4HFROZ,7X,2HEQ,6X,        OUT  186
     46HNUMBER//1X,5HDEG K,5X,5HPOISE,5X,                               OUT  187
     554H------------------ CAL/(CM)(SEC)(K) ------------------,7X,      OUT  188
     610HCAL/(G)(K),7X,25H ---- DIMENSIONLESS -----///)                  OUT  189
C                                                                       OUT  190
C      WRITE DATA                                                       OUT  191
C                                                                       OUT  192
       IF(LEWIS.EQ.0.) GO TO 135                                        OUT  193
       WRITE(6,110) ITT,(ANS(I),I=1,11)                                 OUT  194
  110  FORMAT(I6,F9.0,5HX10-6,F6.0,5HX10-6,F6.0,5HX10-6,F6.0,5HX10-6,   OUT  195
     1F7.0,5HX10-6,F7.0,5HX10-6,F8.4,4F10.4)                            OUT  196
       GO TO 108                                                        OUT  197
  135  WRITE(6,136) ITT,(ANS(I),I=1,10)                                 OUT  198
  136  FORMAT(I6,F9.0,5HX10-6,F6.0,5HX10-6,F6.0,5HX10-6,F6.0,5HX10-6,   OUT  199
     1F7.0,5HX10-6,F7.0,5HX10-6,F8.4,3F10.4)                            OUT  200
       GO TO 108                                                        OUT  201
  104  IF(.NOT.RKT) GO TO 200                                           OUT  202
       IF(LM.EQ.14.OR.LM.EQ.15) GO TO 201                               OUT  203
       IF(RKT.AND.(LM.EQ.27.OR.LM.EQ.28)) GO TO 137                     OUT  204
       IF(RKT.AND.(LM.EQ.40.OR.LM.EQ.41)) GO TO 137                     OUT  205
       IF(RKT.AND.(LM.EQ.53.OR.LM.EQ.54)) GO TO 137                     OUT  206
       GO TO 200                                                        OUT  207
  201  LLL=LLL+1                                                        OUT  208
       GO TO 106                                                        OUT  209
  200  IF(LM-LLL) 112,111,112                                           OUT  210
  111  WRITE(6,113)                                                     OUT  211
  113  FORMAT(1H0)                                                      OUT  212
       LLL=LLL+5                                                        OUT  213
  112  IF(.NOT.FROZN) GO TO 115                                         OUT  214
       WRITE(6,116) ITT,(ANS(I),I=1,4),ANS(7),ANS(9)                    OUT  215
  116  FORMAT(30X,I6,F9.0,3F11.0,F13.4,F10.4)                           OUT  216
       GO TO 108                                                        OUT  217
  115  IF(LEWIS.EQ.0.) GO TO 118                                        OUT  218
       WRITE(6,117) ITT,(ANS(I),I=1,11)                                 OUT  219
  117  FORMAT(I6,F9.0,3F11.0,2F12.0,F13.4,4F10.4)                       OUT  220
       GO TO 108                                                        OUT  221
  118  WRITE(6,119) ITT,(ANS(I),I=1,10)                                 OUT  222
  119  FORMAT(I6,F9.0,3F11.0,2F12.0,F13.4,3F10.4)                       OUT  223
  106  LM=LM+1                                                          OUT  224
       IF(MAXNP.GT.0) GO TO 132                                         OUT  225
  133  CONTINUE                                                         OUT  226
C                                                                       OUT  227
C      PUNCHED CARDS                                                    OUT  228
C                                                                       OUT  229
       IF(.NOT.PUNCH) GO TO 137                                         OUT  230
       IF(RKT.AND.(LM.EQ.15.OR.LM.EQ.16)) GO TO 137                     OUT  231
       IF(RKT.AND.(LM.EQ.28.OR.LM.EQ.29)) GO TO 137                     OUT  232
       IF(RKT.AND.(LM.EQ.41.OR.LM.EQ.42)) GO TO 137                     OUT  233
       IF(RKT.AND.(LM.EQ.54.OR.LM.EQ.55)) GO TO 137                     OUT  234
       PUNCH 121, TT,PP,(ANS(I),I=1,13),FPC                             OUT  235
  121  FORMAT (F8.2,3X,E10.5,4F9.2,2F11.2/F9.5,F10.5,3F9.5,F11.5,3X,    OUT  236
     1 E10.5,2X,F8.4)                                                   OUT  237
  137  CONTINUE                                                         OUT  238
C                                                                       OUT  239
       RETURN                                                           OUT  240
       END                                                              OUT  241
```

```
C
      SUBROUTINE LGRNGE(TT)                                                  LGRN    1
C                                                                            LGRN    2
      COMMON /INTERP/ Z(20),Y(20,3),NTP,ANSR(3)                              LGRN    3
C                                                                            LGRN    4
      DIMENSION A(10)                                                        LGRN    5
C                                                                            LGRN    6
      EQUIVALENCE (XX,A(1)),(X0,A(2)),(X1,A(3)),(X2,A(4)),(X3,A(5)),         LGRN    7
     1(Y0,A(6)),(Y1,A(7)),(Y2,A(8)),(Y3,A(9))                                LGRN    8
C                                                                            LGRN    9
      IF(TT-Z(2))10,10,11                                                    LGRN   10
   10 MX=1                                                                   LGRN   11
      GO TO 51                                                               LGRN   12
   11 IF(TT-Z(NTP-1)) 12,12,13                                               LGRN   13
   13 MX=NTP-3                                                               LGRN   14
      GO TO 51                                                               LGRN   15
   12 K=NTP-1                                                                LGRN   16
      DO 14 JA=2,K                                                           LGRN   17
      IF(TT-Z(JA))15,15,14                                                   LGRN   18
   15 MX=JA-2                                                                LGRN   19
      GO TO 51                                                               LGRN   20
   14 CONTINUE                                                               LGRN   21
   51 XX=ALOG(TT+1.0)                                                        LGRN   22
      DO 22 I=1,4                                                            LGRN   23
      MXI=MX+I-1                                                             LGRN   24
   22 A(I+1)=ALOG(Z(MXI)+1.0)                                                LGRN   25
      B1=((XX-X1)*(XX-X2)*(XX-X3))/(X0-X1)/(X0-X2)/(X0-X3)                   LGRN   26
      B2=((XX-X0)*(XX-X2)*(XX-X3))/(X1-X0)/(X1-X2)/(X1-X3)                   LGRN   27
      B3=((XX-X0)*(XX-X1)*(XX-X3))/(X2-X0)/(X2-X1)/(X2-X3)                   LGRN   28
      B4=((XX-X0)*(XX-X1)*(XX-X2))/(X3-X0)/(X3-X1)/(X3-X2)                   LGRN   29
      DO 8 J=1,3                                                             LGRN   30
      DO 3 I=1,4                                                             LGRN   31
      MXI=MX+I-1                                                             LGRN   32
    3 A(I+5)=ALOG(Y(MXI,J)+1.0)                                              LGRN   33
      ANSWR=B1*Y0+B2*Y1+B3*Y2+B4*Y3                                          LGRN   34
    8 ANSR(J)=EXP(ANSWR)-1.0                                                 LGRN   35
      RETURN                                                                 LGRN   36
      END                                                                    LGRN   37
```

APPENDIX D

SAMPLE PROBLEMS - INPUT AND OUTPUT

Case 51 - Input

```
REACTANTS
N 1.      H 4.      CL1.      C 4.                    72.06   -70690.  S298.15  O
C 1.      H 1.86955C .0312565 .008415                 18.58   -2999.082L298.15  F
AL1.                                                   9.0C     0.0     S298.15  F
MG1.      C 1.                          00             .20              S298.15  F
H 2.      O 1.                                         .16    -68317.4 L298.15  F

OMIT              ALH               AL2O              AL2O2
OMIT              C2                C3                CCL               CCL4
OMIT              CH                CH2               CH4               CN
OMIT              COCL2             CS2               CLCN              CL2O
OMIT              CLO2              MGS               N2O               NS
OMIT              SCL               SCL2              S2CL2             SOCL
OMIT              SOCL2             SO2CL2            SO3
INSERT            AL2O3(L)
NAMELISTS
 $INPT2  KASE=51, RKT=T,PSIA=T,P=500,NODATA=T                $
 $RKTINP PCP=2.5,2.75,3,3.25,3.5,4,10,34.02285, 100,1000,10000     $
```

Case 51 - Output

```
REACTANTS
N   1.0000  H   4.0000  CL  1.0000  O   4.0000      -0.      72.0600     -70690.00  S   298.150  O   -0.
C   1.0000  H   1.8696  O   0.0313  S   0.0084      -0.      18.5800      -2999.08  L   298.150  F   -0.
AL  1.0000      -0.          -0.          -0.         -0.      9.0000         0.     S   298.150  F   -0.
MG  1.0000  O   1.0000       -0.          -0.       00 -0.     0.2000        -0.     S   298.150  F   -0.
H   2.0000  O   1.0000       -0.          -0.         -0.      0.1600     -68317.40  L   298.150  F   -0.
OMIT              ALH               AL2O              AL2O2
OMIT              C2                C3                CCL               CCL4
OMIT              CH                CH2               CH4               CN
OMIT              COCL2             CS2               CLCN              CL2O
OMIT              CLO2              MGS               N2O               NS
OMIT              SCL               SCL2              S2CL2             SOCL
OMIT              SOCL2             SO2CL2            SO3
INSERT            AL2O3(L)
NAMELISTS

$INPT2

KASE  =                51,

T     =    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,
P     =    5.0000000E+02,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,
PSIA  =     T, MMHG  =      F, NSQM  =      F,
V     =    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,
RHO   =    5.0000000E+02,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,
ERATIO=      F, OF    =      F, FPCT  =      F, FA    =      F,
MIX   =    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,
TP    =      F, HP    =      F, SP    =      F, TV    =      F, UV    =      F, SV    =      F,
RKT   =      T, SHOCK =      F, DEIN  =      F, OTTO  =      F, CR    =     0.          , SO    =     0.          , SO    =     0.
IONS  =      F, IDEBUG=                0, TRACE =     0.          , SIUNIT=      F, EUNITS=      F,
TRNSPT=      T, FROZN =      F, PUNCH =      F, NODATA=      T,
$ END
NO INPT2 VALUE GIVEN FOR OF, ERAT, FA, OR FPCT
```

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SPECIES BEING CONSIDERED IN THIS SYSTEM
    J12/65  AL(S)          J12/65  AL(L)          J12/65  AL             J 6/70  ALCL           J 9/64  ALCL2
    J 6/70  ALCL3(S)       J 6/70  ALCL3(L)       J 6/70  ALCL3          J12/62  ALN(S)         J 3/67  ALN
    J 6/70  ALO            J 9/64  ALOCL          J12/67  ALOH           J12/68  ALO2           J12/68  ALO2H
    J 6/70  AL2CL6         J 3/64  AL2O3(S)       J 3/64  AL2O3(L)       J 3/61  C(S)           J 3/61  C
    J12/68  CCL2           J 6/70  CCL3           J 3/61  CH2O           J 6/69  CH3            J 6/66  CNN
    J12/70  CN2            J 9/65  CO             J12/65  COCL           J 3/61  COS            J 9/65  CO2
    J12/62  CS             J12/68  C2CL2          J 3/67  C2H            J 3/61  C2H2           J 9/65  C2H4
    L 5/72  C2H6           J 3/67  C2N            J 3/61  C2N2           J 9/66  C2O            J 6/68  C3O2
    J12/69  C4             J12/69  C5             J 3/61  CL             J 6/61  CLO            J 9/65  CL2
    J 9/65  H              J 3/64  HALO           J 9/64  HCL            L12/69  HCN            J12/70  HCO
    J12/70  HNCO           J 3/63  HNO            J 3/64  HO2            J 3/61  H2             L11/65  H2O(S)
    L11/65  H2O(L)         J 3/61  H2O            L 2/69  H2O2           J12/65  H2S            J 9/62  MG(S)
    J 9/62  MG(L)          J 9/62  MG             J 3/66  MGCL            J12/65  MGCL2(S)       J12/65  MGCL2(L)
    J12/69  MGCL2          J12/66  MGH            J 3/64  MGN            J12/65  MGO(S)         J12/65  MGO(L)
    J12/65  MGO            J 6/67  MGOH           J 6/67  MGO2H2         J12/71  MGS(S)         J 3/61  N
    J12/70  NCO            J12/71  NH             J12/65  NH2            J 9/65  NH3            J 6/63  NO
    J12/65  NOCL           J 9/64  NO2            J12/65  NO2CL          J12/64  NO3            J 9/65  N2
    J12/65  N2H4           J 9/64  N2O4           J12/70  N3             J 6/62  O              J12/70  OH
    J 9/65  O2             J 6/61  O3             J12/65  S(S)           J12/65  S(L)           J 6/71  S
    J 6/67  SH             J 6/61  SN             J 6/71  SO             J 6/61  SO2            J12/65  S2

$RKTINP

EQL   =     T, FROZ  =     T,

SUBAR =   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,

SUPAR =   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,

PCP   =   2.5000000E+00,   2.7500000E+00,   3.0000000E+00,   3.2500000E+00,   3.5000000E+00,   4.0000000E+00,
          1.0000000E+01,   3.4022850E+01,   1.0000000E+02,   1.0000000E+03,   1.0000000E+04,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,

NFZ   =               1,

$ END

OF =   2.579098
                          EFFECTIVE FUEL          EFFECTIVE OXIDANT            MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                    HSUBO
(KG-MOL)(DEG K)/KG      -9.92203147E+02         -0.30277923E+03          -0.24394427E+03

KG-ATOMS/KG                 BOP(I,2)                BOP(I,1)                  BO(I)
       N                 0.                      0.85114220E-02          0.61333306E-02
       H                 0.85409148E-01          0.34045688E-01          0.48396638E-01
       CL                0.                      0.85114220E-02          0.61333306E-02
       O                 0.19127246E-32          0.34045688E-01          0.25067738E-01
       C                 0.45344284E-01          0.                      0.12669193E-01
       S                 0.38157215E-03          0.                      0.10661126E-03
       AL                0.11938507E-01          0.                      0.33356188E-02
       MG                0.17757250E-03          0.                      0.49613757E-04

PT       N        H        CL        O         C         S        AL        MG
 1   -13.569   -9.034   -20.870   -19.840   -11.590   -17.222   -19.688   -21.832   12.000
 2   -13.684   -9.154   -21.372   -20.772   -11.369   -16.985   -21.017   -22.434    3.000
PC/PT= 1.769526    T =  2483.75
 2   -13.685   -9.155   -21.376   -20.779   -11.367   -16.983   -21.028   -22.439    2.000
PC/PT= 1.777143    T =  2481.97
 3   -13.751   -9.225   -21.709   -21.419   -11.185   -16.859   -21.952   -22.866    3.000
 4   -13.769   -9.244   -21.806   -21.609   -11.127   -16.827   -22.228   -22.934    3.000
 4   -13.779   -9.254   -21.789   -21.545   -11.179   -16.842   -22.136   -22.951    3.000
 5   -13.823   -9.297   -21.833   -21.545   -11.266   -16.854   -22.136   -22.952    3.000
 6   -13.863   -9.337   -21.873   -21.546   -11.346   -16.866   -22.135   -22.953    2.000
 7   -13.900   -9.374   -21.910   -21.546   -11.420   -16.878   -22.135   -22.953    2.000
 7   -13.888   -9.363   -21.931   -21.624   -11.356   -16.858   -22.271   -23.006    2.000
 8   -13.913   -9.390   -22.070   -21.900   -11.271   -16.813   -22.745   -23.193    3.000
 9   -14.086   -9.571   -23.143   -24.101   -10.505   -16.605   -26.548   -24.720    4.000
10   -14.323   -9.814   -24.931   -28.009    -8.957   -16.582   -33.289   -27.498    4.000
10   -14.324   -9.815   -24.924   -27.990    -8.963   -16.581   -33.267   -27.788    3.000
11   -14.555  -10.040   -26.870   -32.455    -7.060   -16.744   -40.922   -33.493    4.000
12   -15.152  -10.583   -32.489   -45.990    -0.912   -17.604   -63.504   -50.483    5.000
12   -15.163  -10.598   -32.338   -45.514    -1.232   -17.568   -62.828   -49.968    3.000
13   -16.122  -11.577   -35.546   -51.136    -1.072   -17.937   -74.386   -58.615    5.000
```

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 500.0 PSIA
CASE NO. 51

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	1.00000	H	4.00000	CL	1.00000	O	4.00000	1.00000	-70690.000	S	298.15	-0.
FUEL	C	1.00000	H	1.86955	O	0.03126	S	0.00841	0.66500	-2999.082	L	298.15	-0.
FUEL	AL	1.00000							0.32212	0.	S	298.15	-0.
FUEL	MG	1.00000	O	1.00000					0.00716	-143690.881	S	298.15	-0.
FUEL	H	2.00000	O	1.00000					0.00573	-68317.400	L	298.15	-0.

O/F= 2.5791 PERCENT FUEL= 27.9400 EQUIVALENCE RATIO= 1.9479 REACTANT DENSITY= 0.

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7771	2.5000	2.7500	3.0000	3.2500	3.5000	4.0000	10.000	34.023	100.00	1000.00	10000.0
P, ATM	34.023	19.145	13.609	12.372	11.341	10.469	9.7208	8.5057	3.4023	1.0000	0.3402	0.0340	0.0034
T, DEG K	2727	2482	2341	2315	2315	2315	2299	2246	1900	1504	1222	800	688
RHO, G/CC	3.5172-3	2.1804-3	1.6450-3	1.5123-3	1.3862-3	1.2795-3	1.1963-3	1.0720-3	5.0741-4	1.8841-4	7.8929-5	1.2086-5	1.4933-6
H, CAL/G	-484.8	-613.2	-683.7	-702.6	-719.8	-735.7	-750.4	-776.3	-938.5	-1115.9	-1241.0	-1435.5	-1576.9
S, CAL/(G)(K)	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272	2.5272
M, MOL WT	23.135	23.195	23.218	23.220	23.219	23.217	23.219	23.225	23.249	23.255	23.255	23.320	24.768
(DLV/DLP)T	-1.00268	-1.00138	-1.00088	-1.00082	-1.00085	-1.00088	-1.00085	-1.00070	-1.00015	-1.00001	-1.00000	-1.05592	-1.03953
(DLV/DLT)P	1.0526	1.0284	1.0186	0.	0.	0.	1.0183	1.0153	1.0036	1.0003	1.0000	2.2603	1.9543
CP, CAL/(G)(K)	0.5694	0.5219	0.5088	0.	0.	0.	0.4987	0.4912	0.4579	0.4490	0.4405	2.8904	2.3412
GAMMA (S)	1.1968	1.2081	1.2143	0.9992	0.9992	0.9991	1.2152	1.2178	1.2313	1.2352	1.2407	1.1046	1.1005
SON VEL,M/SEC	1083.1	1036.7	1008.9	910.1	910.1	910.1	1000.3	989.5	914.6	815.0	736.1	561.3	504.1
MACH NUMBER	0.	1.000	1.279	1.484	1.541	1.592	1.490	1.579	2.130	2.820	3.417	5.025	5.997
AE/AT		1.0000	1.0651	1.1070	1.1626	1.2191	1.2674	1.3500	2.2862	5.2207	11.384	66.308	500.74
CSTAR, FT/SEC		5004	5004	5004	5004	5004	5004	5004	5004	5004	5004	5004	5004
CF		0.680	0.846	0.885	0.920	0.950	0.978	1.024	1.278	1.507	1.649	1.849	1.982
IVAC,LB-SEC/LB		193.2	197.8	200.3	203.3	206.1	208.3	211.8	234.3	258.2	274.2	297.9	316.1
ISP, LB-SEC/LB		105.7	131.6	137.7	143.0	147.8	152.0	159.3	198.7	234.3	256.5	287.6	308.3

MOLE FRACTIONS

ALCL	0.00019	0.00004	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.	0.	0.	0.
ALCL2	0.00049	0.00018	0.00009	0.00008	0.00008	0.00008	0.00007	0.00005	0.00000	0.00000	0.	0.	0.
ALCL3	0.00006	0.00004	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00000	0.00000	0.	0.	0.
ALOCL	0.00008	0.00002	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000	0.	0.	0.	0.
ALOH	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.	0.
ALO2H	0.00002	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
AL2O3(S)	0.	0.	0.	0.00504	0.01890	0.03166	0.03723	0.03725	0.03733	0.03733	0.03730	0.03730	0.03730
AL2O3(L)	0.03674	0.03710	0.03721	0.03218	0.01832	0.00556	0.	0.	0.	0.	0.	0.	0.
C(S)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.00266	0.05872
CO	0.26412	0.26332	0.26249	0.26230	0.26229	0.26227	0.26215	0.26172	0.25750	0.24736	0.23225	0.17345	0.07536
COS	0.00005	0.00005	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	0.00006	0.00005	0.00003	0.00002
CO2	0.01814	0.01957	0.02065	0.02087	0.02086	0.02086	0.02100	0.02150	0.02600	0.03613	0.05103	0.10718	0.14921
CS	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.
CL	0.00171	0.00087	0.00054	0.00050	0.00052	0.00054	0.00052	0.00042	0.00008	0.00000	0.00000	0.	0.
H	0.00597	0.00295	0.00180	0.00166	0.00173	0.00180	0.00172	0.00139	0.00024	0.00001	0.00000	0.	0.
HCL	0.13146	0.13342	0.13410	0.13419	0.13416	0.13413	0.13418	0.13437	0.13497	0.13560	0.13702	0.13716	0.13716
HCN	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.
HCO	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
H2	0.32172	0.32472	0.32632	0.32661	0.32659	0.32657	0.32675	0.32739	0.33228	0.34234	0.35701	0.41045	0.39641
H2O	0.14672	0.14552	0.14458	0.14438	0.14435	0.14433	0.14419	0.14374	0.13949	0.12910	0.11331	0.05974	0.07377
H2S	0.00140	0.00166	0.00181	0.00183	0.00181	0.00178	0.00179	0.00185	0.00216	0.00231	0.00233	0.00235	0.00237
MG	0.00002	0.00001	0.00000	0.00000	0.00000	0.00001	0.00000	0.00000	0.00000	0.	0.	0.	0.
MGCL	0.00003	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000	0.	0.	0.
MGCL2	0.00102	0.00107	0.00109	0.00109	0.00109	0.00109	0.00109	0.00109	0.00111	0.00083	0.00007	0.00000	0.
MGO(S)	0.	0.	0.	0.	0.	0.	0.	0.	0.	0.00028	0.00104	0.00111	0.00111
MGOH	0.00003	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000	0.	0.	0.
MGO2H2	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.
NH3	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000	0.00000	0.00001	0.00000
NO	0.00003	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
N2	0.06831	0.06848	0.06854	0.06855	0.06855	0.06854	0.06855	0.06857	0.06863	0.06863	0.06858	0.06857	0.06858
O	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.	0.
OH	0.00071	0.00027	0.00013	0.00012	0.00012	0.00013	0.00012	0.00009	0.00001	0.00000	0.	0.	0.
S	0.00009	0.00005	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00000	0.00000	0.	0.	0.
SH	0.00355	0.00041	0.00033	0.00031	0.00032	0.00033	0.00033	0.00029	0.00010	0.00001	0.00000	0.	0.
SO	0.00016	0.00010	0.00007	0.00006	0.00007	0.00007	0.00007	0.00006	0.00001	0.00000	0.	0.	0.
SO2	0.00007	0.00005	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00001	0.00000	0.00000	0.	0.
S2	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00002	0.00000	0.00000	0.	0.

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	ALCL3(S)	ALCL3(L)	ALN(S)	ALN	ALO	ALO2	AL2CL6
C	CCL2	CCL3	CH2O	CH3	CNN	CN2	COCL	C2CL2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3O2	C4	C5	CLO
CL2	HALO	HNCO	HNO	HO2	H2O(S)	H2O(L)	H2O2	MG(S)	MG(L)
MGCL2(S)	MGCL2(L)	MGH	MGN	MGO(L)	MGO	MGS(S)	N	NCO	NH
NH2	NOCL	NO2	NO2CL	NO3	N2H4	N2O4	N3	O2	O3
S(S)	S(L)	SN							

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

O/F= 2.5791 PERCENT FUEL= 27.9400 EQUIVALENCE RATIO= 1.9479 CHAMBER PRESSURE= 34.023 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	---------- CAL/(CM)(SEC)(K) ----------					CAL/(G)(K)		---- DIMENSIONLESS -----		
2727	778.X10-6	414.X10-6	380.X10-6	795.X10-6	377.X10-6	1171.X10-6	0.4965	0.5992	0.4859	0.3978	2.2923
2482	726.	385.	344.	729.	208.	937.	0.4903	0.5528	0.4880	0.4282	2.2369
2341	695.	369.	322.	691.	137.	828.	0.4862	0.5303	0.4892	0.4456	2.1757
2315	690.	366.	318.	684.	128.	812.	0.4854	0.5272	0.4893	0.4480	2.1613
2315	690.	366.	318.	684.	133.	818.	0.4854	0.5290	0.4893	0.4464	2.1651
2315	690.	366.	318.	685.	138.	823.	0.4854	0.5307	0.4893	0.4449	2.1686
2299	687.	364.	316.	680.	134.	814.	0.4849	0.5290	0.4894	0.4462	2.1601
2246	675.	358.	308.	666.	111.	777.	0.4832	0.5213	0.4898	0.4527	2.1205
1900	599.	319.	254.	573.	27.	601.	0.4704	0.4851	0.4912	0.4836	1.5213
1504	507.	274.	194.	468.	11.	479.	0.4522	0.4677	0.4896	0.4949	0.6759
1222	437.	241.	152.	393.	18.	411.	0.4370	0.4682	0.4855	0.4974	0.6391
800	322.	190.	100.	290.	44.	334.	0.4133	0.5094	0.4585	0.4906	0.6528
688	287.	174.	90.	264.	56.	320.	0.4084	0.5450	0.4444	0.4893	0.6339

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 500.0 PSIA
CASE NO. 51

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	N	1.00000	H	4.00000	CL	1.00000	O	4.00000	1.00000	-70690.000	S	298.15	-0.
FUEL	C	1.00000	H	1.86955	O	0.03126	S	0.00841	0.66500	-2999.082	L	298.15	-0.
FUEL	AL	1.00000							0.32212	0.	S	298.15	-0.
FUEL	MG	1.00000	O	1.00000					0.00716	-143690.881	S	298.15	-0.
FUEL	H	2.00000	O	1.00000					0.00573	-68317.400	L	298.15	-0.

O/F= 2.5791 PERCENT FUEL= 27.9400 EQUIVALENCE RATIO= 1.9479 REACTANT DENSITY= 0.

	CHAMBER	THROAT	EXIT
PC/P	1.0000	1.7885	2.5000
P, ATM	34.023	19.023	13.609
T, DEG K	2727	2451	2303
RHO, G/CC	3.5172-3	2.1887-3	1.6664-3
H, CAL/G	-484.8	-613.9	-682.3
S, CAL/(G)(K)	2.5272	2.5272	2.5272
M, MOL WT	23.135	23.135	23.135
CP, CAL/(G)(K)	0.4697	0.4636	0.4599
GAMMA (S)	1.2238	1.2274	1.2296
SON VEL,M/SEC	1095.2	1039.7	1008.7
MACH NUMBER	0.	1.000	1.275
AE/AT		1.0000	1.1683
CSTAR, FT/SEC		4970	4970
CF		0.686	0.849
IVAC,LB-SEC/LB		192.4	196.7
ISP, LB-SEC/LB		106.0	131.1

MOLE FRACTIONS

ALCL	0.00019	ALCL2	0.00049	ALCL3	0.00006	ALOCL	0.00008
ALOH	0.00001	ALO2H	0.00002	AL2O3(L)	0.03674	CO	0.26412
COS	0.00005	CO2	0.01814	CS	0.00001	CL	0.00171
H	0.00597	HCL	0.13146	HCN	0.00001	HCO	0.00001
H2	0.32172	H2O	0.14672	H2S	0.00140	MG	0.00002
MGCL	0.00003	MGCL2	0.00102	MGOH	0.00003	MGO2H2	0.00001
NH3	0.00001	NO	0.00003	N2	0.06831	O	0.00001
OH	0.00071	S	0.00009	SH	0.00055	SO	0.00016
SO2	0.00007	S2	0.00003				

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

AL(S)	AL(L)	AL	ALCL3(S)	ALCL3(L)	ALN(S)	ALN	ALO	ALO2	AL2CL6
AL2O3(S)	C(S)	C	CCL2	CCL3	CH2O	CH3	CNN	CN2	COCL
C2CL2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2O	C3O2	C4
C5	CLO	CL2	HALO	HNCO	HNO	HO2	H2O(S)	H2O(L)	H2O2
MG(S)	MG(L)	MGCL2(S)	MGCL2(L)	MGH	MGN	MGO(S)	MGO(L)	MGO	MGS(S)
N	NCO	NH	NH2	NOCL	NO2	NO2CL	NO3	N2H4	N2O4
N3	O2	O3	S(S)	S(L)	SN				

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING FROZEN COMPOSITION DURING EXPANSION

O/F= 2.5791 PERCENT FUEL= 27.9400 EQUIVALENCE RATIO= 1.9479 CHAMBER PRESSURE= 34.023 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	CP FROZ	PRANDTL FROZ
DEG K	POISE	----- CAL/(CM)(SEC)(K) ----			CAL/(G)(K)	
2727	778.X10-6	414.X10-6	380.X10-6	795.X10-6	0.4965	0.4859
2451	720.	384.	338.	722.	0.4893	0.4878
2303	688.	367.	315.	682.	0.4848	0.4891

Case 52 - Input

```
REACTANTS
H 2.                                        00         100.    0.         G298.15  F
O 2.                                        0C         100.0   0.0        G298.15  O

NAMELISTS
 $INPT2 KASE=52,DETN=T,ERATIC=T,MIX=1,T=298.15,500, P=1
```

Case 52 - Output

```
REACTANTS
H    2.0000     -0.          -0.          -0.        00 -0.       100.0000           0.    G    298.150  F    -0.
O    2.0000     -0.          -0.          -0.        00 -0.       100.0000           0.    G    298.150  O    -0.
NAMELISTS

$INPT2

KASE   =              52,

T      =   2.9815000E+02,     5.0000000E+02,     0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,

P      =   1.0000000E+00,     0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,

PSIA   =    F, MMHG   =     F, NSQM   =     F,

V      =   0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,

RHO    =   1.0000000E+00,     0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,

ERATIO=     T, OF     =     F, FPCT   =     F, FA     =     F,

MIX    =   1.0000000E+00,     0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,    0.            ,    0.            ,    0.            ,
           0.            ,    0.            ,    0.            ,

TP     =    F, HP     =     F, SP     =     F, TV     =     F, UV     =     F, SV     =     F,

RKT    =    F, SHOCK =      F, DETN   =     T, OTTO   =     F, CR     =   0.            , SO     =   0.            , SO     =   0.

IONS   =    F, IDEBUG=                   0, TRACE =   0.            , SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =      F, PUNCH =      F, NODATA=      F,

$ END

SPECIES BEING CONSIDERED IN THIS SYSTEM
    J 9/65  H                    J 3/64  HO2                J 3/61  H2                 L11/65  H2O(S)             L11/65  H2O(L)
    J 3/61  H2O                  L 2/69  H2O2               J 6/62  O                  J12/70  OH                 J 9/65  O2
    J 6/61  O3

OF =    7.936411
                          EFFECTIVE FUEL            EFFECTIVE OXIDANT            MIXTURE
ENTHALPY                     HPP(2)                      HPP(1)                  HSUBO
(KG-MOL)(DEG K)/KG        0.                        0.                          0.

KG-ATOMS/KG                 BOP(I,2)                   BOP(I,1)                   BO(I)
      H                   0.99209300E+00            0.                          0.11101694E+00
      O                   0.                        0.62502343E-01              0.55508222E-01

DETONATION VELOCITY CALCULATIONS

PT       H         O
 1   -10.312   -15.661     8.000

T EST.= 3611.38
           P/P1                T/T1
   0       0.15000000E+02      0.12112625E+02

PT       H         O
 1   -10.228   -15.582     3.000

PT       H         O
 1   -10.224   -15.583     3.000

PT       H         O
 1   -10.224   -15.583     2.000
 2   -10.327   -15.692     6.000

T EST.= 3728.78
           P/P1                T/T1
   0       0.15000000E+02      0.74575531E+01
 2   -10.434   -15.790     3.000
 2   -10.441   -15.789     3.000
 2   -10.441   -15.788     2.000
```

DETONATION PROPERTIES OF AN IDEAL REACTING GAS

CASE NO. 52

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H 2.00000	1.00000	1405.408	G	500.00	-0.
OXIDANT	O 2.00000	1.00000	1455.140	G	500.00	-0.

O/F= 7.9364 PERCENT FUEL= 11.1902 EQUIVALENCE RATIO= 1.0000 REACTANT DENSITY= 0.

UNBURNED GAS

P1,ATM	1.0000	1.0000
T1,DEG K	298.15	500.00
H1,CAL/G	0.	118.40
M1,MOL WT	12.010	12.010
GAMMA1	1.4015	1.3856
SON VEL,M/SEC	537.8	692.5

BURNED GAS

P, ATM	18.844	10.998
T, DEG K	3683	3607
RHO, G/CC	9.0261-4	5.2888-4
H, CAL/G	679.5	760.9
S, CAL/(G)(K)	4.1589	4.2558
M, MOL WT	14.474	14.235
(DLV/DLP)T	-1.08305	-1.08990
(DLV/DLT)P	2.3791	2.5176
CP, CAL/(G)(K)	3.9365	4.3702
GAMMA (S)	1.1291	1.1268
SON VEL,M/SEC	1545.5	1540.9

DETONATION PARAMETERS

P/P1	18.844	10.998
T/T1	12.352	7.215
M/M1	1.2052	1.1852
RHO/RHO1	1.8386	1.8067
MACH NO.	5.2833	4.0199
DET VEL,M/SEC	2841.5	2783.9

MOLE FRACTIONS

H	0.08139	0.09230
HO2	0.00011	0.00009
H2	0.16475	0.16935
H2O	0.53045	0.50628
H2O2	0.00002	0.00002
O	0.03886	0.04365
OH	0.13496	0.13663
O2	0.04945	0.05169

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

H2O(S) H2O(L) O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

NO TRANSPORT DATA WAS FOUND FOR THE SPECIES HO2

NO TRANSPORT DATA WAS FOUND FOR THE SPECIES H2O2

TRANSPORT PROPERTIES OF THE DETONATED GAS

O/F= 7.9364 PERCENT FUEL= 11.1902 EQUIVALENCE RATIO= 1.0000 FIRST DETONATION PRESSURE= 18.844 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	---------- CAL/(CM)(SEC)(K) ----------					CAL/(G)(K)		---- DIMENSIONLESS -----		
3683	1112.X10-6	707.X10-6	719.X10-6	1426.X10-6	8068.X10-6	9494.X10-6	0.7662	3.9365	0.5979	0.4613	1.3677

NO TRANSPORT DATA WAS FOUND FOR THE SPECIES HO2

NO TRANSPORT DATA WAS FOUND FOR THE SPECIES H2O2

3607	1091.	717.	697.	1414.	9051.	10465.	0.7649	4.3702	0.5900	0.4554	1.3582

Case 122 - Input

```
REACTANTS
N 2.     H 8.     C 2.                    50.     12734.8  L298.15  F  .7861
N 2.     H 4.                             50.     12050.   L298.15  F 1.0036
F 2.                                      100.    -3098.   L 85.02  O 1.505

NAMELISTS
 $INPT2 KASE=122,P=1000,PSIA=T,OF=T,MIX=2.5,  RKT=T, NODATA=T          $
 $RKTINP PCP=10,68.0457, SUBAR=10,5,3.2,1.5,1.1,1.01,1.001,
   SUPAR=1.0005,1.05,1.1,1.5,1.8,2,5,10,100,200,500,1000               $
```

Case 122 - Output

```
REACTANTS
N   2.0000  H   8.0000  C   2.0000     -0.        -0.        50.0000      12734.80  L   298.150  F    0.78610
N   2.0000  H   4.0000     -0.        -0.        -0.        50.0000      12050.00  L   298.150  F    1.00360
F   2.0000     -0.        -0.        -0.        -0.       100.0000      -3098.00  L    85.020  O    1.50500
NAMELISTS

$INPT2

KASE  =              122,

T     =   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,

P     =   1.0000000E+03,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,

PSIA  =    T, MMHG  =     F, NSQM  =     F,

V     =   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,

RHO   =   1.0000000E+03,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,

ERATIO=     F, OF    =     T, FPCT  =     F, FA    =     F,

MIX   =   2.5000000E+00,   0           ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   C           ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,

TP    =     F, HP    =     F, SP    =     F, TV    =     F, UV    =     F, SV    =     F,

RKT   =     T, SHOCK =     F, DETN  =     F, OTTO  =     F, CR    =    0.          , SO    =    0.          , SO    =    0.

IONS  =     F, IDEBUG=                0, TRACE =    0.          , SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =     F, PUNCH =     F, NODATA=     T,

$ END

SPECIES BEING CONSIDERED IN THIS SYSTEM
    J 3/61  C(S)          J 3/61  C           J 6/70  CF          J 6/70  CF2         J 6/69  CF3
    J 6/69  CF4           J12/67  CH          J 6/69  CH2         J 6/69  CH3         J 3/61  CH4
    J 6/69  CN            J 6/66  CNN         J12/70  CN2         J12/69  C2          J12/67  C2F2
    J 6/69  C2F4          J 3/67  C2H         J12/67  C2HF        J 3/61  C2H2        J 9/65  C2H4
    L 5/72  C2H6          J 3/67  C2N         J 3/61  C2N2        J12/69  C3          J12/69  C4
    J12/69  C5            J 9/65  F           J 6/69  FCN         J12/60  F2          J 9/65  H
    L12/69  HCN           J12/68  HF          J 3/61  H2          J 3/61  N           J 6/65  NF
    J 3/64  NF2           J 6/69  NF3         J12/71  NH          J12/65  NH2         J 9/65  NH3
    J 9/65  N2            J12/65  N2H4        J12/70  N3
```

```
$RKTINP

EQL   =     T, FROZ  =     T,

SUBAR =  1.0000000E+01,   5.0000000E+00,   3.0000000E+00,   2.0000000E+00,   1.5000000E+00,   1.1000000E+00,
         1.0100000E+00,   1.0010000E+00,   0.          ,   0.          ,   0.          ,   0.          ,
         0.          ,

SUPAR =  1.0005000E+00,   1.0500000E+00,   1.1000000E+00,   1.5000000E+00,   1.8000000E+00,   2.0000000E+00,
         5.0000000E+00,   1.0000000E+01,   1.0000000E+02,   2.0000000E+02,   5.0000000E+02,   1.0000000E+03,
         0.          ,

PCP   =  1.0000000E+01,   6.8045700E+01,   0.          ,   0.          ,   0.          ,   0.          ,
         0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
         0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
         0.          ,   0.          ,   0.          ,   0.          ,

NFZ   =              1,

$ END

OF =   2.500000

                          EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                  HSUBO
(KG-MOL)(DEG K)/KG       0.14793078E+03          -0.41029893E+02         0.12958869E+02

KG-ATOMS/KG                  BOP(I,2)                BOP(I,1)                BO(I)
        N                 0.47844928E-01          0.                      0.13669979E-01
        H                 0.12896802E+00          0.                      0.36848007E-01
        C                 0.16639085E-01          0.                      0.47540242E-02
        F                 0.                      0.52636011E-01          0.37597151E-01

PT       N         H         C         F
 1  -13.886   -11.179   -5.953   -19.837   10.000
 2  -14.031   -11.466   -5.420   -20.308    4.000
PC/PT= 1.750480   T =  4188.90
 2  -14.030   -11.466   -5.421   -20.307    2.000
PC/PT= 1.749150   T =  4189.27
 3  -14.468   -12.543   -3.483   -21.918    5.000
 3  -14.513   -12.456   -4.065   -21.827    4.000
 4  -15.066   -13.883   -3.603   -23.502    5.000
 5  -13.762   -11.329   -4.452   -20.028    7.000
 5  -13.887   -11.181   -5.950   -19.840    5.000
 5  -13.887   -11.180   -5.951   -19.838    2.000
 5  -13.887   -11.180   -5.951   -19.838    2.000
 5  -13.887   -11.180   -5.951   -19.838    1.000
 5  -13.887   -11.180   -5.951   -19.838    1.000
 6  -13.889   -11.184   -5.945   -19.844    2.000
 6  -13.888   -11.184   -5.945   -19.844    2.000
 6  -13.889   -11.184   -5.945   -19.844    1.000
 7  -13.892   -11.190   -5.934   -19.854    2.000
 7  -13.892   -11.191   -5.931   -19.856    2.000
 7  -13.892   -11.191   -5.931   -19.856    2.000
 8  -13.898   -11.202   -5.910   -19.875    2.000
 8  -13.901   -11.207   -5.901   -19.883    2.000
 8  -13.901   -11.208   -5.900   -19.884    2.000
 8  -13.901   -11.208   -5.900   -19.884    1.000
 9  -13.910   -11.225   -5.866   -19.913    2.000
 9  -13.914   -11.234   -5.851   -19.928    2.000
 9  -13.915   -11.235   -5.849   -19.929    2.000
 9  -13.915   -11.235   -5.849   -19.929    1.000
10  -13.958   -11.319   -5.692   -20.069    3.000
10  -13.959   -11.321   -5.689   -20.071    2.000
10  -13.959   -11.321   -5.689   -20.071    1.000
11  -14.004   -11.411   -5.521   -20.219    3.000
11  -14.003   -11.411   -5.522   -20.218    2.000
12  -14.015   -11.433   -5.480   -20.255    3.000
12  -14.020   -11.444   -5.461   -20.272    2.000
12  -14.021   -11.447   -5.455   -20.277    2.000
12  -14.021   -11.447   -5.455   -20.277    2.000
13  -14.037   -11.481   -5.394   -20.331    3.000
13  -14.037   -11.479   -5.396   -20.329    2.000
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THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 1000.0 PSIA
CASE NO. 122

CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000	H 8.00000	C 2.00000			0.50000	12734.800	L	298.15	0.7861
FUEL	N 2.00000	H 4.00000				0.50000	12050.000	L	298.15	1.0036
OXIDANT	F 2.00000					1.00000	-3098.000	L	85.07	1.5050

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 REACTANT DENSITY= 1.2521

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7491	10.000	68.046	1.0021	1.0084	1.0241	1.0586	1.1181	1.3245	1.5759	1.6895	1.7946
P, ATM	68.046	38.902	6.8046	1.0000	67.906	67.480	65.442	64.279	60.858	51.376	43.178	40.275	37.916
T, DEG K	4464	4189	3502	2902	4463	4460	4452	4435	4408	4324	4239	4206	4177
RHO, G/CC	3.8190-3	2.3626-3	5.1436-4	9.4214-5	3.8123-3	3.7917-3	3.7416-3	3.6369-3	3.4701-3	3.0004-3	2.5841-3	2.4341-3	2.3111-3
H, CAL/G	25.8	-206.2	-825.1	-1381.0	24.9	22.2	15.5	1.3	-22.1	-93.1	-164.3	-192.4	-216.4
S, CAL/(G)(K)	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398
M, MOL WT	20.558	20.877	21.722	22.433	20.559	20.563	20.572	20.591	20.623	20.721	20.819	20.858	20.891
(DLV/DLP)T	-1.03593	-1.02942	-1.02251	-1.00455	-1.03590	-1.03583	-1.03564	-1.03524	-1.03458	-1.03255	-1.03052	-1.02971	-1.02902
(DLV/DLT)P	1.5692	1.4890	1.3681	1.1157	1.5689	1.5681	1.5659	1.5613	1.5537	1.5296	1.5044	1.4941	1.4852
CP, CAL/(G)(K)	1.3378	1.2425	1.9126	0.7232	1.3375	1.3365	1.3341	1.3289	1.3202	1.2922	1.2616	1.2489	1.2377
GAMMA (S)	1.1655	1.1645	1.1051	1.1736	1.1655	1.1655	1.1654	1.1652	1.1650	1.1643	1.1637	1.1636	1.1635
SON VEL,M/SEC	1450.6	1393.3	1217.1	1123.5	1450.4	1449.7	1448.0	1444.6	1438.8	1421.3	1403.6	1396.7	1390.7
MACH NUMBER	0.	1.000	2.192	3.054	0.059	0.120	0.203	0.313	0.440	0.702	0.899	0.967	1.024
AE/AT		1.0000	2.3984	10.183	10.000	5.0000	3.0000	2.0000	1.5000	1.1000	1.0100	1.0010	1.0005
CSTAR, FT/SEC		6872	6872	6872	6872	6872	6872	6872	6872	6872	6872	6872	6872
CF		0.665	1.274	1.638	0.041	0.083	0.140	0.216	0.302	0.476	0.602	0.645	0.680
IVAC,LB-SEC/LB		264.2	323.3	381.8	2145.4	1077.1	655.5	449.7	351.0	279.1	265.5	264.3	264.2
ISP, LB-SEC/LB		142.1	272.1	349.9	8.8	17.7	29.9	46.1	64.5	101.7	128.6	137.8	145.2

MOLE FRACTIONS

C(S)	0.	0.	0.03126	0.08883	0.	0.	0.	0.	0.	0.	0.	0.	0.
C	0.00253	0.00183	0.00046	0.00002	0.00253	0.00252	0.00250	0.00246	0.00238	0.00217	0.00195	0.00187	0.00180
CF	0.01983	0.01805	0.00969	0.00142	0.01982	0.01980	0.01976	0.01966	0.01949	0.01896	0.01840	0.01817	0.01796
CF2	0.00593	0.00636	0.00601	0.00253	0.00593	0.00594	0.00595	0.00597	0.00601	0.00613	0.00627	0.00633	0.00639
CF3	0.00004	0.00004	0.00003	0.00001	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004
CH	0.00024	0.00015	0.00002	0.00000	0.00024	0.00024	0.00024	0.00023	0.00022	0.00019	0.00016	0.00015	0.00014
CH2	0.00001	0.00001	0.00000	0.	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001
CN	0.01306	0.01186	0.03640	0.00080	0.01306	0.01305	0.01301	0.01295	0.01284	0.01248	0.01210	0.01194	0.01180
CN2	0.00001	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000	0.00000
C2	0.00132	0.00115	0.00039	0.00001	0.00132	0.00132	0.00132	0.00131	0.00129	0.00124	0.00119	0.00116	0.00114
C2F2	0.00002	0.00002	0.00001	0.00000	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002
C2H	0.00899	0.00970	0.00652	0.00027	0.00899	0.00900	0.00902	0.00907	0.00914	0.00937	0.00958	0.00966	0.00973
C2HF	0.00041	0.00045	0.00031	0.00032	0.00041	0.00042	0.00042	0.00042	0.00042	0.00043	0.00044	0.00045	0.00045
C2H2	0.00148	0.00161	0.00109	0.00004	0.00149	0.00149	0.00149	0.00150	0.00151	0.00155	0.00159	0.00160	0.00162
C2N	0.00535	0.00571	0.00387	0.00020	0.00535	0.00536	0.00537	0.00539	0.00543	0.00554	0.00565	0.00569	0.00573
C2N2	0.00046	0.00057	0.00064	0.00007	0.00046	0.00046	0.00047	0.00047	0.00048	0.00051	0.00055	0.00056	0.00057
C3	0.00179	0.00253	0.00301	0.00008	0.00179	0.00180	0.00181	0.00185	0.00192	0.00213	0.00237	0.00248	0.00257
C4	0.00001	0.00002	0.00002	0.00000	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00002
C5	0.00001	0.00001	0.00004	0.00000	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001
F	0.08241	0.06744	0.03443	0.01527	0.08236	0.08218	0.08176	0.08084	0.07935	0.07476	0.07016	0.06834	0.06678
FCN	0.00159	0.00158	0.00118	0.00031	0.00159	0.00159	0.00159	0.00159	0.00159	0.00158	0.00158	0.00158	0.00158
F2	0.00001	0.00000	0.00000	0.00000	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00000	0.00000	0.00000
H	0.04706	0.03628	0.01447	0.00308	0.04702	0.04689	0.04659	0.04593	0.04485	0.04155	0.03823	0.03693	0.03581
HCN	0.01297	0.01322	0.01003	0.00176	0.01297	0.01298	0.01299	0.01300	0.01303	0.01311	0.01319	0.01321	0.01323
HF	0.65661	0.68449	0.73343	0.74638	0.65672	0.65704	0.65784	0.65953	0.66232	0.67085	0.67943	0.68282	0.68573
H2	0.01410	0.01087	0.00422	0.00079	0.01408	0.01404	0.01395	0.01375	0.01343	0.01243	0.01145	0.01106	0.01073
N	0.00034	0.00019	0.00003	0.00000	0.00034	0.00034	0.00033	0.00032	0.00031	0.00026	0.00022	0.00020	0.00019
NH	0.00001	0.00001	0.00000	0.00000	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001	0.00001
NH	0.00002	0.00001	0.00000	0.00000	0.00002	0.00002	0.00002	0.00002	0.00002	0.00001	0.00001	0.00001	0.00001
N2	0.12337	0.12583	0.13244	0.13810	0.12338	0.12341	0.12347	0.12362	0.12386	0.12461	0.12537	0.12568	0.12594

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

CF4	CH3	CH4	CNN	C2F4	C2H4	C2H6	NF2	NF3	NH2
NH3	N2H4	N3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

3	-14.104	-11.622	-5.136	-20.556	3.000
3	-14.104	-11.621	-5.139	-20.553	2.000
4	-14.138	-11.697	-5.001	-20.672	3.000
5	-14.306	-12.093	-4.291	-21.270	4.000
5	-14.297	-12.071	-4.331	-21.237	3.000
5	-14.297	-12.071	-4.331	-21.236	1.000
6	-14.392	-12.323	-3.880	-21.604	3.000
6	-14.411	-12.288	-4.123	-21.567	3.000
6	-14.380	-12.238	-4.140	-21.490	3.000
6	-14.380	-12.238	-4.140	-21.489	2.000
7	-14.458	-12.365	-4.097	-21.687	3.000
7	-14.430	-12.318	-4.113	-21.615	3.000
7	-14.430	-12.318	-4.113	-21.615	2.000
8	-14.840	-13.108	-3.842	-22.744	5.000
8	-14.818	-13.055	-3.860	-22.677	3.000
8	-14.818	-13.055	-3.860	-22.677	1.000
9	-15.061	-13.859	-3.610	-23.485	4.000
9	-15.061	-13.855	-3.611	-23.482	2.000
10	-15.575	-18.484	-2.366	-28.630	9.000
10	-15.583	-18.553	-2.339	-28.855	2.000
11	-15.726	-19.815	-1.909	-33.294	3.000
11	-15.717	-19.735	-1.933	-32.997	1.000
12	-15.912	-21.559	-1.477	-40.206	2.000
12	-15.923	-21.664	-1.456	-40.645	1.000
13	-16.126	-23.640	-1.141	-49.285	2.000
13	-16.113	-23.512	-1.157	-48.706	1.000

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 1000.0 PSIA
CASE NO. 122

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000 H 8.00000 C 2.00000	0.50000	12734.800	L	298.15	0.7861
FUEL	N 2.00000 H 4.00000	0.50000	12050.000	L	298.15	1.0036
OXIDANT	F 2.00000	1.00000	-3098.000	L	85.02	1.5050

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 REACTANT DENSITY= 1.2521

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7491	2.4253	2.6616	4.9633	6.6292	7.7306	26.846	66.440	1448.42	3724.92	13047.0	33844.8
P, ATM	68.046	38.902	29.263	25.566	13.710	10.265	8.8021	2.5347	1.0242	0.0470	0.0183	0.0052	0.0020
T, DEG K	4464	4189	4055	3992	3709	3608	3569	3224	2911	1625	1301	955	748
RHO, G/CC	3.8190-3	2.3626-3	1.8497-3	1.6469-3	9.6438-4	7.4680-4	6.4949-4	2.1203-4	9.6152-5	8.0299-6	3.8999-6	1.5169-6	7.4686-7
H, CAL/G	25.8	-206.2	-317.5	-368.8	-593.1	-690.8	-741.7	-1126.4	-1374.8	-1982.6	-2102.7	-2225.1	-2295.6
S, CAL/(G)(K)	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398
M, MOL WT	20.558	20.877	21.031	21.102	21.410	21.541	21.609	22.131	22.427	22.793	22.794	22.794	22.795
(DLV/DLP)T	-1.03593	-1.02932	-1.02614	-1.02468	-1.01853	-1.02754	-1.02563	-1.01183	-1.00469	-1.00004	-1.00000	-1.00000	-1.00000
(DLV/DLT)P	1.5692	1.4890	1.4465	1.4262	1.3332	1.6866	1.6420	1.3053	1.1195	1.0014	1.0000	1.0000	1.0000
CP, CAL/(G)(K)	1.3378	1.2425	1.1874	1.1600	1.0258	2.2124	2.1000	1.2323	0.7338	0.3809	0.3626	0.3448	0.3352
GAMMA (S)	1.1655	1.1635	1.1633	1.1634	1.1659	1.1002	1.1019	1.1265	1.1719	1.2978	1.3166	1.3384	1.3515
SON VEL,M/SEC	1450.6	1393.3	1365.6	1352.7	1295.9	1237.8	1230.1	1168.2	1124.6	877.1	790.5	682.8	607.2
MACH NUMBER	0.	1.000	1.241	1.343	1.756	1.978	2.060	2.658	3.044	4.674	5.339	6.356	7.259
AE/AT		1.0000	1.0500	1.1000	1.5000	1.8000	2.0000	5.0000	10.000	100.00	200.00	500.00	1000.00
CSTAR, FT/SEC		6872	6872	6872	6872	6872	6872	6872	6872	6872	6872	6872	6872
CF		0.665	0.809	0.867	1.086	1.169	1.210	1.482	1.634	1.957	2.015	2.072	2.104
IVAC,LB-SEC/LB		264.2	259.3	273.6	296.6	307.7	313.7	356.4	381.2	432.8	441.8	450.7	455.7
ISP, LB-SEC/LB		142.1	172.8	185.3	232.0	249.7	258.4	316.6	349.1	418.0	430.3	442.6	449.4

MOLE FRACTIONS

C(S)	0.	0.	0.	0.	0.	0.00883	0.01766	0.07021	0.08855	0.09425	0.09428	0.09428	0.09428
C	0.00253	0.00183	0.00151	0.00137	0.00081	0.00064	0.00057	0.00014	0.00007	0.	0.	0.	0.
CF	0.01983	0.01805	0.01706	0.01657	0.01414	0.01247	0.01139	0.00442	0.00148	0.00000	0.	0.	0.
CF2	0.00593	0.00636	0.00665	0.00680	0.00772	0.00742	0.00686	0.00361	0.00253	0.00006	0.00000	0.	0.
CF3	0.00004	0.00004	0.00004	0.00004	0.00004	0.00004	0.00003	0.00001	0.00001	0.00000	0.00000	0.	0.
CF4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00382	0.00387	0.00387	0.00387
CH	0.00024	0.00015	0.00011	0.00009	0.00004	0.00003	0.00003	0.00000	0.00000	0.	0.	0.	0.
CH2	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
CN	0.01306	0.01186	0.01117	0.01083	0.00910	0.00806	0.00743	0.00295	0.00084	0.	0.	0.	0.
CN2	0.00301	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
C2	0.00132	0.00115	0.00105	0.00100	0.00076	0.00061	0.00052	0.00009	0.00001	0.	0.	0.	0.
C2F2	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00002	0.00000	0.00000	0.	0.	0.	0.
C2H	0.00899	0.00970	0.00998	0.01009	0.01013	0.00923	0.00815	0.00204	0.00029	0.	0.	0.	0.
C2HF	0.00041	0.00045	0.00047	0.00048	0.00052	0.00047	0.00040	0.00010	0.00001	0.	0.	0.	0.
C2H2	0.00148	0.00161	0.00167	0.00170	0.00179	0.00160	0.00139	0.00033	0.00005	0.	0.	0.	0.
C2N	0.00535	0.00571	0.00587	0.00594	0.00615	0.00551	0.00486	0.00124	0.00022	0.	0.	0.	0.
C2N2	0.00046	0.00057	0.00064	0.00067	0.00089	0.00086	0.00077	0.00026	0.00008	0.	0.	0.	0.
C3	0.00179	0.00253	0.00300	0.00324	0.00457	0.00439	0.00384	0.00082	0.00009	0.	0.	0.	0.
C4	0.00001	0.00002	0.00002	0.00002	0.00003	0.00003	0.00002	0.00000	0.00000	0.	0.	0.	0.
C5	0.00001	0.00001	0.00002	0.00003	0.00006	0.00006	0.00005	0.00001	0.00000	0.	0.	0.	0.
F	0.08241	0.06744	0.06021	0.05688	0.04236	0.03891	0.03670	0.02478	0.01549	0.00003	0.00000	0.	0.
FCN	0.00159	0.00158	0.00158	0.00158	0.00160	0.00149	0.00136	0.00062	0.00031	0.00000	0.	0.	0.
F2	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
H	0.04706	0.03628	0.03112	0.02877	0.01888	0.01629	0.01564	0.00889	0.00321	0.00000	0.	0.	0.
HCN	0.01297	0.01372	0.01329	0.01331	0.01324	0.01233	0.01145	0.00524	0.00183	0.00000	0.00000	0.	0.
HF	0.65661	0.68449	0.69794	0.70412	0.73071	0.73527	0.73436	0.73644	0.74610	0.76072	0.76074	0.76074	0.76074
H2	0.01410	0.01087	0.00935	0.00866	0.00579	0.00495	0.00468	0.00242	0.00082	0.00000	0.00000	0.	0.
N	0.00034	0.00019	0.00014	0.00012	0.00005	0.00004	0.00004	0.00001	0.00000	0.	0.	0.	0.
NF	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
NH	0.00002	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.	0.	0.	0.
N2	0.12337	0.12583	0.12708	0.12767	0.13037	0.13135	0.13175	0.13535	0.13803	0.14111	0.14111	0.14111	0.14111

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

CH3	CH4	CNN	C2F4	C2H4	C2H6	NF2	NF3	NH2	NH3
N2H4	N3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 CHAMBER PRESSURE= 68.046 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		DIMENSIONLESS		
4464	1431.X10-6	580.X10-6	354.X10-6	935.X10-6	2979.X10-6	3914.X10-6	0.4281	1.3369	0.6556	0.4889	1.5016
4189	1373.	536.	338.	874.	2606.	3480.	0.4251	1.2416	0.6676	0.4898	1.5520
3502	1219.	445.	288.	733.	1558.	2292.	0.4162	0.9554	0.6918	0.5082	1.6400
2902	1072.	382.	233.	615.	619.	1235.	0.4057	0.6440	0.7065	0.5590	1.7130
4463	1431.	580.	354.	934.	2978.	3912.	0.4281	1.3365	0.6556	0.4889	1.5018
4460	1430.	579.	354.	934.	2974.	3908.	0.4280	1.3356	0.6557	0.4889	1.5024
4452	1429.	578.	354.	932.	2964.	3896.	0.4279	1.3332	0.6561	0.4889	1.5038
4435	1425.	575.	353.	928.	2944.	3872.	0.4278	1.3280	0.6568	0.4889	1.5068
4408	1419.	571.	351.	922.	2909.	3831.	0.4275	1.3193	0.6580	0.4889	1.5118
4324	1402.	558.	346.	904.	2798.	3701.	0.4266	1.2913	0.6617	0.4890	1.5272
4239	1384.	544.	341.	885.	2679.	3564.	0.4256	1.2607	0.6654	0.4894	1.5428
4206	1377.	539.	339.	878.	2631.	3509.	0.4253	1.2480	0.6669	0.4897	1.5490
4177	1370.	534.	337.	872.	2588.	3460.	0.4249	1.2368	0.6681	0.4899	1.5543
4053	1344.	516.	329.	845.	2399.	3244.	0.4236	1.1865	0.6735	0.4914	1.5762
3992	1330.	506.	325.	832.	2297.	3129.	0.4228	1.1590	0.6762	0.4926	1.5869
3709	1265.	465.	306.	772.	1806.	2577.	0.4193	1.0244	0.6877	0.5029	1.6221
3603	1242.	454.	298.	752.	1661.	2413.	0.4179	0.9848	0.6905	0.5071	1.6283
3569	1234.	451.	294.	745.	1626.	2372.	0.4173	0.9751	0.6909	0.5073	1.6326
3224	1154.	418.	263.	681.	1162.	1842.	0.4116	0.8306	0.6978	0.5203	1.6763
2911	1074.	383.	234.	617.	634.	1251.	0.4058	0.6492	0.7062	0.5572	1.7133
1625	678.	238.	103.	340.	3.	343.	0.3706	0.3740	0.7386	0.7395	0.8626
1301	561.	196.	68.	264.	0.	264.	0.3570	0.3571	0.7577	0.7577	0.8896
955	424.	148.	35.	183.	0.	183.	0.3403	0.3403	0.7910	0.7910	
748	336.	117.	19.	136.	0.	136.	0.3324	0.3324	0.8214	0.8214	

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 1000.0 PSIA
CASE NO. 122

CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000	H 8.00000	C 2.00000			0.50000	12734.800	L	298.15	0.7861
FUEL	N 2.00000	H 4.00000				0.50000	12050.000	L	298.15	1.0036
OXIDANT	F 2.00000					1.00000	-3098.000	L	85.07	1.5050

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 REACTANT DENSITY= 1.2521

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.8302	10.000	68.046	1.0022	1.0091	1.0261	1.0634	1.1280	1.3545	1.6348	1.7619	1.8817
P, ATM	68.046	37.178	6.8046	1.0000	67.894	67.435	66.317	63.991	60.323	50.238	41.623	38.620	36.162
T, DEG K	4464	4891	2621	1635	4462	4455	4438	4402	4344	4168	3993	3925	3867
RHO, G/CC	3.8190-3	2.3936-3	6.5049-4	1.5322-4	3.8124-3	3.7924-3	3.7437-3	3.6416-3	3.4790-3	3.0201-3	2.6116-3	2.4649-3	2.3430-3
H, CAL/G	25.8	-218.0	-746.3	-1134.6	24.8	21.9	14.7	-0.6	-25.5	-100.8	-175.0	-203.6	-228.4
S, CAL/(G)(K)	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398
M, MOL WT	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558
CP, CAL/(G)(K)	0.4281	0.4233	0.4061	0.3774	0.4280	0.4280	0.4278	0.4276	0.4271	0.4257	0.4242	0.4236	0.4230
GAMMA (S)	1.2917	1.2960	1.3124	1.3419	1.2917	1.2918	1.2919	1.2921	1.2925	1.2938	1.2951	1.2957	1.2962
SON VEL,M/SEC	1527.1	1428.2	1179.4	942.0	1526.7	1525.6	1522.8	1516.8	1506.9	1476.7	1446.2	1434.2	1423.8
MACH NUMBER	0.	1.000	2.155	3.309	0.059	0.118	0.200	0.309	0.435	0.697	0.896	0.966	1.024
AE/AT		1.0000	2.0675	7.1598	10.000	5.0000	3.0000	2.0000	1.5000	1.1000	1.0100	1.0010	1.0005
CSTAR, FT/SEC		6617	6617	6617	6617	6617	6617	6617	6617	6617	6617	6617	6617
CF		0.708	1.260	1.545	0.044	0.089	0.151	0.233	0.325	0.510	0.643	0.687	0.723
IVAC,LB-SEC/LB		258.0	301.7	339.4	2061.0	1037.5	632.4	434.7	340.3	272.0	259.2	258.1	258.1
ISP, LB-SEC/LB		145.6	259.2	317.8	9.1	18.4	31.0	47.9	66.8	104.9	132.2	141.3	148.7

MOLE FRACTIONS

C	0.00253	CF	0.01983	CF2	0.00593	CF3	0.00004	
CH	0.00024	CH2	0.00001	CH	0.01306	CN2	0.00001	
C2	0.00132	C2F2	0.00002	C2H	0.00899	C2HF	0.00041	
C2H2	0.00148	C2N	0.00535	C2N2	0.00046	C3	0.00179	
C4	0.00001	C5	0.00001	F	0.08241	FCN	0.00159	
F2	0.00001	H	0.04706	HCN	0.01297	HF	0.65661	
H2	0.01410	N	0.00034	NF	0.00001	NH	0.00002	
N2	0.12337							

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C(S)	CF4	CH3	CH4	CNN	C2F4	C2H4	C2H6	NF2	NF3
NH2	NH3	N2H4	N3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 1000.0 PSIA
CASE NO. 122

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	8.00000	C	2.00000	0.50000	12734.800	L	298.15	0.7861
FUEL	N	2.00000	H	4.00000			0.50000	12050.000	L	298.15	1.0036
OXIDANT	F	2.00000					1.00000	-3098.000	L	85.02	1.5050

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 REACTANT DENSITY= 1.2521

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.8302	2.4922	2.8860	5.6856	7.8973	9.4581	39.876	111.17	3103.65	8387.46	31078.1	83508.0
P, ATM	68.046	37.178	27.303	23.578	11.968	8.6163	7.1944	1.7064	0.6121	0.0219	0.0081	0.0022	0.0008
T, DEG K	4464	3891	3626	3505	2995	2772	2656	1871	1441	577	433	297	222
RHO, G/CC	3.8190-3	2.3936-3	1.8866-3	1.6851-3	1.0013-3	7.7882-4	6.7870-4	2.2849-4	1.0641-4	9.5246-6	4.6894-6	1.8494-6	9.1778-7
H, CAL/G	25.8	-218.0	-330.1	-380.7	-593.3	-684.8	-732.1	-1044.2	-1207.5	-1513.6	-1561.8	-1607.5	-1632.1
S, CAL/(G)(K)	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398	2.7398
M, MOL WT	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558	20.558
CP, CAL/(G)(K)	0.4281	0.4233	0.4207	0.4194	0.4126	0.4089	0.4067	0.3872	0.3721	0.3382	0.3351	0.3327	0.3313
GAMMA (S)	1.2917	1.2960	1.2983	1.2995	1.3059	1.3096	1.3117	1.3327	1.3509	1.4003	1.4054	1.4096	1.4119
SON VEL,M/SEC	1527.1	1428.2	1379.8	1357.3	1257.6	1211.6	1187.0	1004.2	887.4	571.5	496.3	411.2	356.4
MACH NUMBER	0.	1.000	1.251	1.359	1.810	2.013	2.122	2.980	3.620	6.280	7.343	8.990	10.451
AE/AT		1.0000	1.0500	1.1000	1.5000	1.8000	2.0000	5.0000	10.000	100.00	200.00	500.00	1000.00
CSTAR, FT/SEC		6617	6617	6617	6617	6617	6617	6617	6617	6617	6617	6617	6617
CF		0.708	0.856	0.914	1.128	1.209	1.249	1.484	1.593	1.779	1.807	1.833	1.847
IVAC,LB-SEC/LB		258.0	262.6	266.4	286.2	295.5	300.3	330.9	346.1	372.6	376.6	380.3	382.3
ISP, LB-SEC/LB		145.6	176.0	188.1	232.1	248.7	256.8	305.1	327.6	366.0	371.7	377.0	379.8

MOLE FRACTIONS

C	0.00253	CF	0.01983	CF2	0.00593	CF3	0.00004	
CH	0.00024	CH2	0.00001	CN	0.01306	CN2	0.00001	
C2	0.00132	C2F2	0.00002	C2H	0.00899	C2HF	0.00041	
C2H2	0.00148	C2N	0.00535	C2N2	0.00046	C3	0.00179	
C4	0.00001	C5	0.00001	F	0.68241	FCN	0.00159	
F2	0.00001	H	0.04706	HCN	0.01297	HF	0.65661	
H2	0.01410	N	0.00034	NF	0.00001	NH	0.00002	
N2	0.12337							

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C(S)	CF4	CH3	CH4	CNN	C2F4	C2H4	C2H6	NF2	NF3
NH2	NH3	N2H4	N3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING FROZEN COMPOSITION DURING EXPANSION

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 CHAMBER PRESSURE= 68.046 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	CP FROZ	PRANDTL FROZ
DEG K	POISE	----- CAL/(CM)(SEC)(K) ----			CAL/(G)(K)	
4464	1431.X10-6	580.X10-6	354.X10-6	935.X10-6	0.4281	0.6556
3891	1295.	524.	309.	833.	0.4233	0.6579
2621	965.	388.	199.	587.	0.4051	0.6674
1635	666.	265.	103.	368.	0.3794	0.6870
4462	1431.	580.	354.	934.	0.4281	0.6556
4455	1429.	579.	354.	933.	0.4280	0.6556
4438	1425.	578.	352.	930.	0.4279	0.6557
4402	1417.	574.	350.	924.	0.4276	0.6558
4344	1403.	569.	345.	914.	0.4271	0.6560
4168	1362.	551.	331.	883.	0.4257	0.6567
3993	1320.	534.	317.	852.	0.4242	0.6574
3925	1303.	527.	312.	839.	0.4236	0.6577
3867	1289.	521.	307.	829.	0.4231	0.6580
3626	1230.	497.	288.	785.	0.4207	0.6591
3505	1199.	485.	278.	762.	0.4194	0.6598
2995	1067.	430.	233.	663.	0.4127	0.6638
2772	1007.	405.	213.	618.	0.4089	0.6658
2656	974.	392.	202.	594.	0.4068	0.6670
1871	743.	297.	126.	423.	0.3872	0.6802
1441	601.	239.	83.	322.	0.3721	0.6946
577	264.	102.	13.	115.	0.3382	0.7741
433	200.	77.	6.	83.	0.3351	0.8025
297	137.	53.	2.	55.	0.3327	0.8360
222	103.	39.	0.	40.	0.3314	0.8539

Case 123 - Input

```
REACTANTS
N 2.     H 4.                                          50.     12050.   L298.15  F 1.0036
N 2.     H 8.     C 2.                                 50.     12734.8  L298.15  F  .7861
F 2.                                                   10C.     -3098.  L  85.02 O 1.505

NAMELIST
 $INPT2  KASE=123,  HP=T,OF=T,MIX=2.5,P=100,10,1, PUNCH=T, NODATA=T  $
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Case 123 - Output

```
REACTANTS
N   2.0000  H   4.0000     -0.         -0.         -0.         50.0000      12050.00  L   298.150  F     1.00360
N   2.0000  H   8.0000  C   2.0000     -0.         -0.         50.0000      12734.80  L   298.150  F     0.78610
F   2.0000     -0.         -0.         -0.         -0.        100.0000      -3098.00  L    85.020  O     1.50500
NAMELIST

$INPT2

KASE   =              123,

T      =    0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,

P      =    1.0000000E+02,  1.0000000E+01,  1.0000000E+00,  0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,

PSIA   =      F, MMHG   =     F, NSQM   =     F,

V      =    0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,

RHO    =    1.0000000E+02,  1.0000000E+01,  1.0000000E+00,  0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,

ERATIO=      F, OF     =     T, FPCT   =     F, FA     =     F,

MIX    =    2.5000000E+00,  0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
            0.          ,   0.          ,   0.          ,

TP     =      F, HP     =     T, SP     =     F, TV     =     F, UV     =     F, SV     =     F,

RKT    =      F, SHOCK =      F, DETN   =     F, OTTO   =     F, CR     =   0.          , SO     =   0.          , SO     =   0.

IONS   =      F, IDEBUG=                     0, TRACE =    0.          , SIUNIT=     F, EUNITS=     F,

TRNSPT=       T, FROZN =      F, PUNCH =      T, NODATA=     T,

$ END

OF =    2.500000
                            EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                       HPP(2)                    HPP(1)                  HSURO
(KG-MOL)(DEG K)/KG          0.14793078E+03          -0.41029893E+02          0.12958869E+02

KG-ATOMS/KG                   BOP(I,2)                  BOP(I,1)                  BO(I)
        N                   0.47844928E-01           0.                      0.13669979E-01
        H                   0.12896802E+00           0.                      0.36848007E-01
        C                   0.16639085E-01           0.                      0.47540242E-02
        F                   0.                       0.52636011E-01          0.37597151E-01

PT      N        H         C        F
 1  -13.724  -11.002   -6.011  -19.566   10.000
 2  -14.692  -12.080   -5.639  -21.205    4.000
 3  -15.657  -13.207   -5.224  -22.881    4.000
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THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED PRESSURES

CASE NO. 123

	CHEMICAL FORMULA						WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2.00000	H	4.00000			0.50000	12050.000	L	298.15	1.0036
FUEL	N	2.00000	H	8.00000	C	2.00000	0.50000	12734.800	L	298.15	0.7861
OXIDANT	F	2.00000					1.00000	-3098.000	L	85.02	1.5050

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 REACTANT DENSITY= 1.2521

THERMODYNAMIC PROPERTIES

P, ATM	100.00	10.000	1.0000
T, DEG K	45..	4118	3733
RHO, G/CC	5.5516-3	5.9440-4	6.3939-5
H, CAL/G	25.8	25.8	25.8
S, CAL/(G)(K)	2.7027	2.9274	3.1582
M, MOL WT	20.658	20.086	19.586
(DLV/DLP)T	-1.03428	-1.04434	-1.05388
(DLV/DLT)P	1.5332	1.7670	2.0318
CP, CAL/(G)(K)	1.2639	1.7797	2.4735
GAMMA (S)	1.1691	1.1484	1.1305
SON VEL,M/SEC	1460.7	1399.2	1338.5

MOLE FRACTIONS

C	0.00228	0.00386	0.00538
CF	0.01984	0.01889	0.01659
CF2	0.00670	0.00325	0.00162
CF3	0.00006	0.00001	0.00000
CH	0.00026	0.00017	0.00009
CH2	0.00001	0.00000	0.00000
CH3	0.00001	0.00000	0.00000
CN	0.01270	0.01433	0.01474
CN2	0.00001	0.00000	0.00000
C2	0.00122	0.00177	0.00213
C2F2	0.00002	0.00001	0.00000
C2H	0.00882	0.00931	0.00876
C2HF	0.00048	0.00020	0.00008
C2H2	0.00163	0.00091	0.00047
C2N	0.00536	0.00501	0.00425
C2N2	0.00051	0.00028	0.00015
C3	0.00158	0.00309	0.00529
C4	0.00001	0.00001	0.00002
C5	0.00001	0.00001	0.00001
F	0.07885	0.09876	0.11566
FCN	0.00177	0.00091	0.00047
F2	0.00001	0.00000	0.00000
H	0.04346	0.06588	0.08820
HCN	0.01370	0.00969	0.00655
HF	0.66208	0.62986	0.60034
H2	0.01454	0.01159	0.00837
N	0.00035	0.00030	0.00022
NF	0.00002	0.00000	0.00000
NH	0.00002	0.00001	0.00000
N2	0.12372	0.12188	0.12061

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C(S)	CF4	CH4	CNN	C2F4	C2H4	C2H6	NF2	NF3	NH2
NH3	N2H4	N3							

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES AT ASSIGNED PRESSURES

O/F= 2.5000 PERCENT FUEL= 28.5714 EQUIVALENCE RATIO= 1.4859 ENTHALPY= 25.8 CAL/G

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		DIMENSIONLESS		
4535	1448.X10-6	581.X10-6	363.X10-6	944.X10-6	2772.X10-6	3716.X10-6	0.4285	1.2628	0.6577	0.4922	1.5088
4118	1346.	573.	316.	889.	4068.	4957.	0.4258	1.7791	0.6447	0.4830	1.4402
3733	1247.	561.	273.	835.	5434.	6269.	0.4231	2.4729	0.6320	0.4919	1.8439

Case 679 - Input

```
REACTANTS
LI1.                                         1.   MO.     S298.15  F
F 2.                                      .5556  M-3098.   L 85.02  0 1.505

NAMELISTS
 $INPT2 KASE=679,          RKT=T,P=1000,PSIA=T,IONS=T,TRNSPT=F          $
 $RKTINP PCP=3,10,30,68.0457,  100,1000,3000,30000,300000               $
```

Case 679 - Output

```
REACTANTS
LI  1.0000     -0.         -0.         -0.         -0.        1.0000  M       0.    S   298.150  F   -0.
F   2.0000     -0.         -0.         -0.         -0.        0.5556  M   -3098.00  L    85.020  O    1.50500
NAMELISTS

$INPT2

KASE  =             679,

T     =    0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,

P     =    1.0000000E+03,   0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0            ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,

PSIA  =     T, MMHG  =     F, NSQM  =     F,

V     =    0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,

RHO   =    1.0000000E+03,   0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,

ERATIO=     F, OF    =     F, FPCT  =     F, FA    =     F,

MIX   =    0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.          ,    0.           ,    0.           ,

TP    =     F, HP    =     F, SP    =     F, TV    =     F, UV    =     F, SV    =     F,

RKT   =     T, SHOCK =     F, DETN  =     F, OTTO  =     F, CR    =    0.            , SO    =    0.            , SO    =    0.

IONS  =     T, IDEBUG=               0, TRACE =    0.            , SIUNIT=     F, EUNITS=     F,

TRNSPT=     F, FROZN =     F, PUNCH =     F, NODATA=     F,

$ END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

SPECIES BEING CONSIDERED IN THIS SYSTEM
    L02/67  E              J 9/65  F              J12/71  F-             J12/60  F2             J 6/62  LI(S)
    J 6/62  LI(L)          J 6/62  LI             J 3/65  LI+            J12/68  LIF(S)         J12/68  LIF(L)
    J12/68  LIF            J12/68  LIF2-          J 6/62  LI2            J12/68  LI2F2          J12/68  LI3F3
```

```
$RKTINP

EQL   =     T, FROZ  =     T,

SUBAR =   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,

SUPAR =   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,

PCP   =   3.0000000E+00,   1.0000000E+01,   3.0000000E+01,   6.8045700E+01,   1.0000000E+02,   1.0000000E+03,
          3.0000000E+03,   3.0000000E+04,   3.0000000E+05,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,   0.          ,   0.          ,
          0.          ,   0.          ,   0.          ,   0.          ,

NFZ   =               1,

$ END

OF =  3.042372
                          EFFECTIVE FUEL          EFFECTIVE OXIDANT            MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                    HSUBO
(KG-MOL)(DEG K)/KG        0.                      -0.41029892E+02           -0.30879939E+02

KG-ATOMS/KG                  BOP(I,2)                BOP(I,1)                  BO(I)
      LI                  0.14411298E+00          0.                        0.35650596E-01
      F                   0.                      0.52636011E-01            0.39614941E-01
      E                   0.                      0.                        0.

PT      LI       F        E
 1  -16.252  -19.930   -9.124    9.000

THE TEMPERATURE=  0.5691E+04 IS OUT OF RANGE FOR POINT    1
 2  -16.576  -20.312   -9.754    4.000

THE TEMPERATURE=  0.5340E+04 IS OUT OF RANGE FOR POINT    2
PC/PT= 1.759768   T =  5340.15
 2  -16.574  -20.310   -9.752    2.000

THE TEMPERATURE=  0.5341E+04 IS OUT OF RANGE FOR POINT    2
PC/PT= 1.755775   T =  5341.50
 3  -16.905  -20.677  -10.381    4.000

THE TEMPERATURE=  0.5036E+04 IS OUT OF RANGE FOR POINT    3
 4  -17.756  -21.506  -11.953    4.000
 5  -18.757  -22.227  -13.740    4.000
 6  -19.856  -22.650  -15.650    4.000
 7  -20.610  -22.760  -16.956    4.000
 8  -28.682  -22.382  -31.023    6.000
 9  -32.281  -22.431    4.000
10  -38.057  -23.151  -41.159    5.000
11  -43.101  -24.151    4.000

                THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC =  1000.0 PSIA
CASE NO.     679

                                                                          MOLES       ENERGY    STATE   TEMP     DENSITY
        CHEMICAL FORMULA                                                            CAL/MOL           DEG K    G/CC
FUEL    LI 1.00000                                                        1.00000       0.        S    298.15   -0.
OXIDANT F  2.00000                                                        0.55560   -3098.000     L     85.02    1.5050

              O/F=  3.0424    PERCENT FUEL= 24.7379    EQUIVALENCE RATIO=  0.8999    REACTANT DENSITY=  0.

                    CHAMBER   THROAT    EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT
PC/P                 1.0000    1.7558    3.0000   10.000    30.000    68.046   130.00    1000.00   3000.00   30000.0   300000.0
P, ATM              68.046    38.755    22.682    6.8046    2.2682    1.0000    0.6805    0.0680    0.0227    0.0023    0.0002
T, DEG K             5691      5341      5036      4421      3909      3511      3300      2091      1809      1495      1301
RHO, G/CC         3.1975-3  1.9826-3  1.2554-3  4.4700-4  1.7400-4  8.6917-5  6.3246-5  1.0160-5  4.0263-6  5.2528-7  6.4894-8
H, CAL/G            -61.4     -339.4    -583.3   -1067.2   -1442.5   -1685.9   -1789.7   -2267.0   -2429.9   -2703.9   -2920.2
S, CAL/(G)(K)       2.7095    2.7095    2.7095    2.7095    2.7095    2.7095    2.7095    2.7095    2.7095    2.7095    2.7095

M, MOL WT          21.943    22.422    22.870    23.837    24.604    25.040    25.170    25.614    26.350    28.401    30.536
(DLV/DLP)T       -1.08263  -1.07304  -1.06368  -1.04207  -1.02213  -1.00871  -1.00433  -1.01420  -1.03902  -1.08732  -1.11244
(DLV/DLT)P         2.0657    1.9966    1.9164    1.6822    1.4008    1.1699    1.0839    1.2038    1.6499    2.7673    3.6211
CP, CAL/(G)(K)     1.6397    1.5925    1.5273    1.2939    0.9518    0.6260    0.4909    0.5744    1.1636    2.8527    4.3303
GAMMA (S)          1.1807    1.1748    1.1699    1.1632    1.1688    1.1973    1.2264    1.2218    1.1593    1.1117    1.0924
SON VEL,M/SEC      1595.6    1525.4    1463.5    1339.5    1242.5    1181.4    1156.3    910.5     813.5     697.4     622.0
MACH NUMBER          0.        1.000     1.428     2.166     2.736     3.121     3.289     4.718     5.473     6.742     7.863

AE/AT                          1.0000    1.1528    2.3321    5.1126    9.4372   12.574    69.284   168.72    1224.37   9528.08
CSTAR, FT/SEC                   7480      7480      7480      7480      7480      7480      7480      7480      7480      7480
CF                             0.669     0.917     1.273     1.491     1.617     1.668     1.884     1.953     2.063     2.145
IVAC,LB-SEC/LB                 288.0     302.4     350.1     386.3     408.2     417.0     454.2     467.0     489.0     506.1
ISP, LB-SEC/LB                 155.6     213.1     295.8     346.7     376.0     387.8     438.1     454.0     479.5     498.8
```

MOLE FRACTIONS

E	0.00294	0.00237	0.00188	0.00096	0.00036	0.00009	0.00003	0.	0.	0.	0.
F	0.21151	0.19574	0.18087	0.14865	0.12245	0.10760	0.10329	0.10154	0.10446	0.11258	0.12105
F-	0.00464	0.00364	0.00284	0.00148	0.00067	0.00028	0.00015	0.00000	0.	0.00000	0.
F2	0.00002	0.00001	0.00001	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
LI	0.12106	0.10422	0.08820	0.05320	0.02455	0.00824	0.00347	0.00000	0.	0.	0.
LI+	0.00758	0.00601	0.00471	0.00243	0.00104	0.00038	0.00019	0.00000	0.	0.	0.
LIF	0.65089	0.68690	0.72056	0.79259	0.85030	0.88273	0.89207	0.88385	0.85238	0.76605	0.67705
LI2	0.00028	0.00014	0.00007	0.00001	0.00000	0.00000	0.00000	0.	0.	0.	0.
LI2F2	0.00109	0.00096	0.00085	0.00068	0.00062	0.00068	0.00081	0.01449	0.04246	0.11762	0.19413
LI3F3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00011	0.00071	0.00374	0.00777

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

LI(S) LI(L) LIF(S) LIF(L) LIF2-

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION

PC = 1000.0 PSIA
CASE NO. 679

	CHEMICAL FORMULA	MOLES	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	LI 1.00000	1.00000	0.	S	298.15	-0.
OXIDANT	F 2.00000	0.55560	-3098.000	L	85.02	1.5050

O/F= 3.0424 PERCENT FUEL= 24.7379 EQUIVALENCE RATIO= 0.8999 REACTANT DENSITY= 0.

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.8444	3.0000	10.000	30.000	68.046	100.00	1000.00	3000.00	30000.0	300000.0
P, ATM	68.046	36.893	22.682	6.8046	2.2682	1.0000	0.6805	0.0680	0.0227	0.0023	0.0002
T, DEG K	5691	4915	4366	3235	2448	1984	1796	984	734	388	195
RHO, G/CC	3.1975-3	2.0071-3	1.3892-3	5.6249-4	2.4781-4	1.3480-4	1.0131-4	1.8501-5	8.2678-6	1.5643-6	3.1113-7
H, CAL/G	-61.4	-354.9	-559.1	-970.7	-1251.7	-1415.4	-1481.3	-1762.9	-1847.8	-1961.3	-2020.0
S, CAL/(G)(K)	2.7095	2.7095	2.7095	2.7095	2.7095	2.7095	2.7095	2.7095	2.7095	2.7095	2.7095
M, MOL WT	21.943	21.943	21.943	21.943	21.943	21.943	21.943	21.943	21.943	21.943	21.943
CP, CAL/(G)(K)	0.3823	0.3746	0.3690	0.3594	0.3544	0.3516	0.3503	0.3421	0.3365	0.3159	0.2915
GAMMA (S)	1.3104	1.3188	1.3253	1.3369	1.3432	1.3470	1.3487	1.3600	1.3683	1.4019	1.4508
SON VEL,M/SEC	1681.0	1567.3	1480.7	1280.1	1116.1	1006.2	958.1	711.9	616.7	453.8	327.4
MACH NUMBER	0.	1.000	1.378	2.155	2.828	3.345	3.598	5.300	6.269	8.786	12.367
AE/AT		1.0000	1.1095	2.0273	4.0221	6.9325	9.0081	45.060	98.405	504.34	2497.35
CSTAR, FT/SEC		7191	7191	7191	7191	7191	7191	7191	7191	7191	7191
CF		0.715	0.931	1.259	1.440	1.536	1.573	1.722	1.764	1.819	1.847
IVAC,LB-SEC/LB		281.0	290.8	326.6	351.8	366.0	371.6	394.9	401.6	410.3	414.7
ISP, LB-SEC/LB		159.8	208.1	281.3	321.8	343.2	351.5	384.8	394.3	406.6	412.8

MOLE FRACTIONS

E	0.00294	F	0.21151	F-	0.00464	F2	0.00002	
LI	0.12106	LI+	0.00758	LIF	0.65089	LI2	0.00028	
LI2F2	0.00109							

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

LI(S) LI(L) LIF(S) LIF(L) LIF2- LI3F3

Case 950 - Input

```
REACTANTS
H 2.                                        100.    0.       G298.15  F
N 1.561760 .419590AR.009324C .000300        100.    -28.2    G298.15  0

OMIT            C2H4            C3U2            H2O(S)          C(S)
OMIT            C2N2            H2O(L)          C2G             C2H2
OMIT            HO2             H2O2
OMIT            NH2             CH2             CH              NH3
OMIT            C2N             CH3             NO2             CH4
OMIT            HCN             C2H             C3              N2O
OMIT            N2C             C2              CN              HCO
OMIT            N2H4            N2O4            CN2
NAMELISTS
 $INPT2 TP=T,P=.1,.01,ERATIO=T,MIX=1.5,1,2, T=3000,2000,KASE=950      $
```

Case 950 - Output

```
REACTANTS
H   2.0000     -0.          -0.          -0.          -0.       100.0000          0.    G   298.150  F   -0.
N   1.5618  0   0.4196  AR  0.0093  C   0.0003       -0.       100.0000       -28.20   G   298.150  0   -0.
OMIT            C2H4            C3O2            H2O(S)          C(S)
OMIT            C2N2            H2O(L)          C2O             C2H2
OMIT            HO2             H2O2
OMIT            NH2             CH2             CH              NH3
OMIT            C2N             CH3             NO2             CH4
OMIT            HCN             C2H             C3              N2O
OMIT            N2C             C2              CN              HCO
OMIT            N2H4            N2O4            CN2
NAMELISTS

$INPT2

KASE  =              950,

T     =    3.0000000E+03,    2.0000000E+03,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

P     =    1.0000000E-01,    1.0000000E-02,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

PSIA  =     F, MMHG  =     F, NSQM  =     F,

V     =    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

RHO   =    1.0000000E-01,    1.0000000E-02,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

ERATIO=     T, OF    =     F, FPCT  =     F, FA    =     F,

MIX   =    1.5000000E+00,    1.0000000E+00,    2.0000000E+00,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

TP    =     T, HP    =     F, SP    =     F, TV    =     F, UV    =     F, SV    =     F,

RKT   =     F, SHOCK =     F, DETN  =     F, OTTO  =     F, CR    =    0.          , SO    =    0.          , SO    =    0.

IONS  =     F, IDEBUG=                0, TRACE =    0.          , SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =     F, PUNCH =     F, NODATA=     F,

$ END

SPECIES BEING CONSIDERED IN THIS SYSTEM
    L 5/66  AR              J 3/61  C               J 3/61  CH2O            J 6/66  CNN             J 9/65  CO
    J 9/65  CO2             L 5/72  C2H6            J12/69  C4              J12/69  C5              J 9/65  H
    J12/70  HNCO            J 3/63  HNO             J 3/61  H2              J 3/61  H2O             J 3/61  N
    J12/70  NCO             J12/71  NH              J 6/63  NO              J12/64  NO3             J 9/65  N2
    J12/70  N3              J 6/62  O               J12/70  OH              J 9/65  O2              J 6/61  O3

OF =  22.849901
                          EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                  HSUBO
(KG-MOL)(DEG K)/KG        0.                      -0.48994914E+00         -0.46940611E+00

KG-ATOMS/KG                  BOP(I,2)                BOP(I,1)                BO(I)
       H                  0.99209300E+00          0.                      0.41597364E-01
       N                  0.                      0.53920039E-01          0.51659231E-01
       O                  0.                      0.14486419E-01          0.13879019E-01
       AR                 0.                      0.32191274E-03          0.30841529E-03
       C                  0.                      0.10357553E-04          0.99232720E-05

PT      H         N         O         AR        C
 1  -12.567   -15.738   -18.416   -29.654   -26.227   17.000
 2  -11.844   -14.915   -21.829   -28.570   -23.639    7.000
 3  -14.101   -17.003   -19.689   -32.185   -27.408    5.000
 4  -13.602   -16.067   -21.821   -30.875   -25.954    8.000
```

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

CASE NO. 950

CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL H 2.00000	1.00000	0.	G	298.15	-0.
OXIDANT N 1.56176 O 0.41959 AR 0.00932 C 0.00030	1.00000	-28.200	G	298.15	-0.

O/F= 22.8499 PERCENT FUEL= 4.1929 EQUIVALENCE RATIO= 1.5000 REACTANT DENSITY= 0.

THERMODYNAMIC PROPERTIES

P, ATM	0.1000	0.1000	0.0100	0.0100
T, DEG K	3000	2000	3000	2000
RHO, G/CC	7.1132-6	1.2964-5	5.6618-7	1.2930-6
H, CAL/G	1551.2	-117.7	3222.6	-103.6
S, CAL/(G)(K)	3.6980	3.0712	4.5486	3.2936
M, MOL WT	17.510	21.275	13.937	21.220
(DLV/DLP)T	-1.08647	-1.00060	-1.08691	-1.00193
(DLV/DLT)P	2.6852	1.0172	2.6389	1.0556
CP, CAL/(G)(K)	4.2389	0.4965	4.9243	0.6014
GAMMA (S)	1.1193	1.2408	1.1296	1.2071
SON VEL,M/SEC	1262.7	984.8	1421.8	972.6

MOLE FRACTIONS

AR	0.00540	0.00656	0.00430	0.00654
CO	0.00016	0.00015	0.00013	0.00015
CO2	0.00002	0.00006	0.00000	0.00007
H	0.18282	0.00196	0.39418	0.00616
H2	0.13549	0.14675	0.06299	0.14483
H2O	0.11209	0.29458	0.01459	0.29282
N	0.00003	0.	0.00008	0.
NO	0.00971	0.00003	0.00767	0.00009
N2	0.44742	0.54952	0.35612	0.54805
O	0.04229	0.00000	0.11840	0.00004
OH	0.05041	0.00039	0.03043	0.00122
O2	0.01417	0.00000	0.01110	0.00003

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C	CH2O	CNN	C2H6	C4	C5	HNCO	HNO	NCO	NH
NO3	N3	O3							

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES AT ASSIGNED TEMPERATURE AND PRESSURE

O/F= 22.8499 PERCENT FUEL= 4.1929 EQUIVALENCE RATIO= 1.5000 FIRST PRESSURE= 0.100 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	---------- CAL/(CM)(SEC)(K) ----------					CAL/(G)(K)		---- DIMENSIONLESS -----		
3000	839.X10-6	563.X10-6	285.X10-6	848.X10-6	10172.X10-6	11020.X10-6	0.4838	4.2389	0.4789	0.3227	1.5462
2000	640.	255.	227.	482.	151.	633.	0.4499	0.4965	0.5971	0.5021	3.0156
3000	808.	829.	173.	1003.	10027.	11029.	0.4968	4.9243	0.4003	0.3608	1.1220
2000	640.	258.	226.	484.	475.	959.	0.4501	0.6014	0.5951	0.4014	2.9182

UF = 34.291058

ENTHALPY	EFFECTIVE FUEL HPP(2)	EFFECTIVE OXIDANT HPP(1)	MIXTURE HSUBO
(KG-MOL)(DEG K)/KG	0.	-0.48994914E+00	-0.47606605E+00

KG-ATOMS/KG	BOP(I,2)	BOP(I,1)	BO(I)
H	0.99209300E+00	0.	0.28111739E-01
N	0.	0.53920039E-01	0.52392171E-01
O	0.	0.14486419E-01	0.14075934E-01
AR	0.	0.32191274E-03	0.31279108E-03
C	0.	0.10357553E-04	0.10064063E-04

PT	H	N	O	AR	C	
1	-12.809	-15.669	-18.085	-29.513	-26.456	5.000
2	-13.412	-14.836	-18.557	-28.413	-28.927	7.000
3	-14.309	-16.920	-19.494	-32.017	-27.442	5.000
4	-14.200	-15.991	-19.315	-30.721	-29.806	8.000

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

CASE NO. 950

CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY \ CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL H 2.00000	1.00000	0.	G	298.15	-0.
OXIDANT N 1.56176 O 0.41959 AR 0.00932 C 0.00030	1.00000	-28.200	G	298.15	-0.

O/F= 34.2911 PERCENT FUEL= 2.8336 EQUIVALENCE RATIO= 1.0000 REACTANT DENSITY= 0.

THERMODYNAMIC PROPERTIES

P, ATM	0.1000	0.1000	0.0100	0.0100
T, DEG K	3000	2000	3000	2000
RHO, G/CC	8.0798-6	1.4956-5	6.6021-7	1.4877-6
H, CAL/G	1372.4	-193.6	2659.6	-166.6
S, CAL/(G)(K)	3.3290	2.7344	4.0132	2.9347
M, MOL WT	19.890	24.545	16.252	24.415
(DLV/DLP)T	-1.07939	-1.00143	-1.07450	-1.00352
(DLV/DLT)P	2.5496	1.0454	2.4081	1.1093
CP, CAL/(G)(K)	3.4784	0.5174	3.7121	0.6795
GAMMA (S)	1.1202	1.2042	1.1319	1.1681
SON VEL,M/SEC	1185.3	903.2	1318.0	891.9

MOLE FRACTIONS

AR	0.00622	0.00768	0.00508	0.00764
CO	0.00017	0.00002	0.00016	0.00004
CO2	0.00003	0.00023	0.00001	0.00021
H	0.14373	0.00041	0.32026	0.00186
H2	0.08374	0.00638	0.04158	0.01318
H2O	0.09639	0.33736	0.01170	0.32680
N	0.00003	0.	0.00009	0.
NO	0.01448	0.00077	0.01013	0.00114
N2	0.51378	0.64260	0.42063	0.63900
O	0.05885	0.00010	0.14391	0.00048
OH	0.05514	0.00212	0.03004	0.00453
O2	0.02743	0.00233	0.01640	0.00513

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C	CH2O	CNN	C2H6	C4	C5	HNCO	HNO	NCO	NH
NO3	N3	O3							

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES AT ASSIGNED TEMPERATURE AND PRESSURE

O/F= 34.2911 PERCENT FUEL= 2.8336 EQUIVALENCE RATIO= 1.0000 FIRST PRESSURE= 0.100 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		DIMENSIONLESS		
3000	855.X10-6	467.X10-6	240.X10-6	707.X10-6	8287.X10-6	8995.X10-6	0.4271	3.4784	0.5164	0.3307	1.6400
2000	661.	206.	186.	391.	194.	585.	0.3988	0.5174	0.6739	0.5849	1.6634
3000	830.	682.	157.	838.	7227.	8065.	0.4369	3.7121	0.4326	0.3820	1.1502
2000	660.	208.	186.	394.	507.	901.	0.3990	0.6795	0.6686	0.4980	1.8302

OF = 17.133338

	EFFECTIVE FUEL HPP(2)	EFFECTIVE OXIDANT HPP(1)	MIXTURE HSUBO
ENTHALPY (KG-MOL)(DEG K)/KG	0.	-0.48994914E+00	-0.46292989E+00

KG-ATOMS/KG	BOP(I,2)	BOP(I,1)	BO(I)
H	0.99209300E+00	0.	0.54710996E-01
N	0.	0.53920039E-01	0.50946508E-01
O	0.	0.14486419E-01	0.13687535E-01
AR	0.	0.32191274E-03	0.30416020E-03
C	0.	0.10357553E-04	0.97863643E-05

PT	H	N	O	AR	C	
1	-12.415	-15.802	-18.700	-29.785	-26.048	5.000
2	-11.566	-14.984	-22.522	-28.708	-22.917	7.000
3	-13.976	-17.075	-19.854	-32.329	-27.382	5.000
4	-12.723	-16.137	-22.515	-31.014	-25.231	8.000

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

CASE NO. 950

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H 2.00000	1.00000	0.	G	298.15	-0.
OXIDANT	N 1.56176 O 0.41959 AR 0.00932 C 0.00030	1.00000	-28.200	G	298.15	-0.

O/F= 17.1333 PERCENT FUEL= 5.5147 EQUIVALENCE RATIO= 2.0000 REACTANT DENSITY= 0.

THERMODYNAMIC PROPERTIES

P, ATM	0.1000	0.1000	0.0100	0.0100
T, DEG K	3000	2000	3000	2000
RHO, G/CC	6.3311-6	1.1450-5	4.9731-7	1.1414-6
H, CAL/G	1774.4	-27.3	3769.9	-8.9
S, CAL/(G)(K)	4.0682	3.3911	5.0648	3.6441
M, MOL WT	15.585	18.790	12.242	18.732
(DLV/DLP)T	-1.08791	-1.00072	-1.09489	-1.00226
(DLV/DLT)P	2.7067	1.0201	2.7866	1.0636
CP, CAL/(G)(K)	4.7915	0.5595	6.0360	0.6904
GAMMA (S)	1.1199	1.2437	1.1286	1.2071
SON VEL,M/SEC	1338.8	1049.1	1516.4	1035.1

MOLE FRACTIONS

AR	0.00474	0.00572	0.00372	0.00570
CO	0.00314	0.00015	0.00012	0.00015
CO2	0.00001	0.00003	0.00000	0.00003
H	0.21280	0.00259	0.44687	0.00813
H2	0.18358	0.25589	0.08095	0.25266
H2O	0.11428	0.25670	0.01589	0.25530
N	0.00003	0.	0.00008	0.
NO	0.00685	0.00001	0.00605	0.00004
N2	0.39356	0.47864	0.38878	0.47715
O	0.03183	0.00000	0.10033	0.00002
OH	0.04415	0.00026	0.02923	0.00081
O2	0.00802	0.00000	0.00797	0.00001

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

C	CH2O	CNN	C2H6	C4	C5	HNCO	HNO	NCO	NH
NO3	N3	O3							

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES AT ASSIGNED TEMPERATURE AND PRESSURE

O/F= 17.1333 PERCENT FUEL= 5.5147 EQUIVALENCE RATIO= 2.0000 FIRST PRESSURE= 0.100 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		DIMENSIONLESS		
3000	820.X10-6	653.X10-6	325.X10-6	978.X10-6	11644.X10-6	12622.X10-6	0.5393	4.7915	0.4524	0.3114	1.5103
2000	621.	302.	263.	565.	204.	769.	0.4996	0.5595	0.5484	0.4516	3.0043
3000	787.	954.	189.	1143.	12426.	13569.	0.5550	6.0360	0.3822	0.3502	1.1004
2000	621.	306.	262.	568.	638.	1206.	0.4999	0.6904	0.5463	0.3552	2.9504

Case 1207 - Input

```
REACTANTS
H 2.                              00       0.050  M          G 300.00
O 2.                              00       0.050  M          G 300.00
AR1.                              00       0.900  M          G 300.00

NAMELISTS
 $INPT2 KASE=1207,P=10,20,MMHG=T, SHOCK=T                    $
 $SHKINP U1=1000,1100,1200,1250,1300,1350,1400,1450,1500, INCDEQ=T,INCDFZ=T $
```

Case 1207 - Output

```
REACTANTS
H   2.0000     -0.          -0.          -0.       00 -0.        0.0500  M      -0.    G   300.000      -0.
O   2.0000     -0.          -0.          -0.       00 -0.        0.0500  M      -0.    G   300.000      -0.
AR  1.0000     -0.          -0.          -0.       00 -0.        0.9000  M      -0.    G   300.000      -0.
NAMELISTS

$INPT2

KASE  =              1207,

T     =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,

P     =    1.0000000E+01,    2.0000000E+01,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

PSIA  =     F, MMHG  =     T, NSQM  =     F,

V     =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,
           0.           ,

RHO   =    1.0000000E+01,    2.0000000E+01,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

ERATIO=     F, OF    =     F, FPCT  =     F, FA    =     F,

MIX   =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

TP    =     F, HP    =     F, SP    =     F, TV    =     F, UV    =     F, SV    =     F,

RKT   =     F, SHOCK =     T, DETN  =     F, OTTO  =     F, CR    =    0.           , SO    =    0.           , SO    =    0.

IONS  =     F, IDEBUG=                0, TRACE =    0.           , SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =     F, PUNCH =     F, NODATA=     F,

$ END

NO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT

SPECIES BEING CONSIDERED IN THIS SYSTEM
    L 5/66  AR              J 9/65  H              J 3/64  HO2             J 3/61  H2              L11/65  H2O(S)
    L11/65  H2O(L)          J 3/61  H2O            L 2/69  H2O2            J 6/62  O               J12/70  OH
    J 9/65  O2              J 6/61  O3

$SHKINP

U1    =    1.0000000E+03,    1.1000000E+03,    1.2000000E+03,    1.2500000E+03,    1.3000000E+03,    1.3500000E+03,
           1.4000000E+03,    1.4500000E+03,    1.5000000E+03,    0.           ,    0.           ,    0.           ,
           0.           ,

MACH1 =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,

GAMMA1=    0.           , INCDEQ=     T, REFLEQ=     F, INCDFZ=     T, REFLFZ=     F, A1    =    1.0000000E+00,

$ END

OF =   0.

                          EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                      HPP(2)                  HPP(1)                  HSUBO
(KG-MOL)(DEG K)/KG        0.                      0.                      0.

KG-ATOMS/KG                  BOP(I,2)                BOP(I,1)                BO(I)
       H                  0.26557648E-02          0.                      0.26557648E-02
       O                  0.26557648E-02          0.                      0.26557648E-02
       AR                 0.23901883E-01          0.                      0.23901883E-01
```

SHOCK WAVE PARAMETERS ASSUMING
EQUILIBRIUM COMPOSITION FOR INCIDENT SHOCKED CONDITIONS

CASE NO. 1207

	CHEMICAL FORMULA	MOLES	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H 2.00000	0.05000	13.478	G	300.00	-0.
FUEL	O 2.00000	0.05000	12.892	G	300.00	-0.
FUEL	AR 1.00000	0.90000	9.191	G	300.00	-0.

O/F= 0. PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.5000 REACTANT DENSITY= 0.

INITIAL GAS (1)

MACH NO.	3.0480	3.3528	3.6576	3.8100	3.9624	4.1148	4.2672	4.4196	4.5720
U1, M/SEC	1000.00	1100.00	1200.00	1250.00	1300.00	1350.00	1400.00	1450.00	1500.00
P, ATM	0.0132	0.0263	0.0263	0.0263	0.0263	0.0263	0.0263	0.0263	0.0263
T, DEG K	300	300	300	300	300	300	300	300	300
RHO, G/CC	2.0126-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5
H, CAL/G	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
S, CAL/(G)(K)	1.2406	1.2041	1.2041	1.2041	1.2041	1.2041	1.2041	1.2041	1.2041
M, MOL WT	37.654	37.654	37.654	37.654	37.654	37.654	37.654	37.654	37.654
CP, CAL/(G)(K)	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372
GAMMA (S)	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249
SON VEL,M/SEC	328.1	328.1	328.1	328.1	328.1	328.1	328.1	328.1	328.1

DID NOT CONVERGE FOR U1= 1000.00 ANSWERS PROBABLY NOT RELIABLE, SOLUTION MAY NOT EXIST

SHOCKED GAS (2)--INCIDENT--EQUILIBRIUM

U2, M/SEC	575.88	667.74	576.55	560.68	549.47	540.62	532.79	525.22	517.53
P, ATM	0.1145	0.2152	0.3235	0.3686	0.4139	0.4604	0.5086	0.5590	0.6118
T, DEG K	1542	1527	1817	1933	2044	2153	2259	2361	2457
RHO, G/CC	3.4949-5	6.6310-5	8.3781-5	8.9742-5	9.5234-5	1.0052-4	1.0577-4	1.1113-4	1.1667-4
H, CAL/G	93.6	91.6	132.6	149.4	166.1	183.1	200.6	218.6	237.1
S, CAL/(G)(K)	1.3281	1.2943	1.2979	1.3001	1.3026	1.3052	1.3080	1.3109	1.3139
M, MOL WT	38.619	38.619	38.614	38.608	38.597	38.580	38.552	38.510	38.453
(DLV/DLP)T	-1.00001	-1.00000	-1.00005	-1.00010	-1.00021	-1.00041	-1.00073	-1.00123	-1.00193
(DLV/DLT)P	1.0003	1.0002	1.0018	1.0037	1.0070	1.0124	1.0208	1.0330	1.0493
CP, CAL/(G)(K)	0.1404	0.1401	0.1442	0.1477	0.1530	0.1611	0.1726	0.1882	0.2078
GAMMA (S)	1.5792	1.5807	1.5582	1.5410	1.5173	1.4865	1.4501	1.4111	1.3733
SON VEL,M/SEC	724.0	721.0	780.8	800.8	817.4	830.6	840.6	848.1	854.2
P2/P1	5.915	8.178	12.294	14.008	15.729	17.495	19.328	21.243	23.247
T2/T1	4.428	5.092	6.057	6.442	6.815	7.178	7.531	7.870	8.191
M2/M1	1.0256	1.0256	1.0255	1.0253	1.0251	1.0246	1.0238	1.0227	1.0212
RHO2/RHO1	1.7365	1.6473	2.0814	2.2294	2.3659	2.4971	2.6277	2.7607	2.8984
V2(U1-U2)M/SEC	424.12	432.26	623.45	689.32	750.53	809.38	857.21	924.78	982.47

MOLE FRACTIONS

AR	9.2306-1	9.2306-1	9.2294-1	9.2280-1	9.2255-1	9.2213-1	9.2146-1	9.2047-1	9.1910-1
H	1.4775-7	7.1348-8	4.3013-6	1.5667-5	4.7564-5	1.2521-4	2.9107-4	6.0405-4	1.1305-3
HO2	9.8099-9	1.0364-8	6.7804-8	1.2217-7	2.0224-7	3.1325-7	4.5774-7	6.3422-7	8.3714-7
H2	3.0708-6	1.8670-6	3.5421-5	8.9393-5	1.9761-4	3.9339-4	7.1392-4	1.1893-3	1.8303-3
H2O	5.1238-2	5.1249-2	5.1028-2	5.0786-2	5.0385-2	4.9758-2	4.8834-2	4.7553-2	4.5891-2
H2O2	7.212-10	9.131-10	4.464 -9	7.362 -9	1.131 -8	1.642 -8	2.267 -8	2.984 -8	3.758 -8
O	3.3010-6	2.0013-6	3.9835-5	1.0212-4	2.2910-4	4.6321-4	8.5589-4	1.4579-3	2.3083-3
OH	7.8598-5	5.9618-5	4.1738-4	7.6735-4	1.2923-3	2.0296-3	2.9976-3	4.1846-3	5.5478-3
O2	2.5621-2	2.5626-2	2.5532-2	2.5439-2	2.5299-2	2.5103-2	2.4848-2	2.4539-2	2.4187-2

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-08 FOR ALL ASSIGNED CONDITIONS

H2O(S) H2O(L) O3

TRANSPORT PROPERTIES OF THE SHOCKED GAS ASSUMING EQUILIBRIUM COMPOSITION

O/F= 0. PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.5000 FIRST SHOCK PRESSURE= 0.1145 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		DIMENSIONLESS		
1542	723.X10-6	140.X10-6	13.X10-6	153.X10-6	1.X10-6	154.X10-6	0.1396	0.1404	0.6600	0.6581	1.5041
1527	719.	139.	13.	152.	1.	153.	0.1395	0.1401	0.6602	0.6590	1.4339
1817	807.	156.	16.	173.	8.	181.	0.1405	0.1442	0.6570	0.6436	1.8061
1933	842.	163.	18.	181.	18.	198.	0.1408	0.1477	0.6558	0.6268	1.9897
2044	874.	169.	19.	188.	35.	223.	0.1411	0.1530	0.6545	0.5992	2.1791
2153	906.	176.	20.	196.	65.	261.	0.1413	0.1611	0.6530	0.5595	2.3617
2259	936.	182.	21.	203.	113.	316.	0.1416	0.1726	0.6512	0.5112	2.5206
2361	965.	188.	22.	211.	182.	393.	0.1418	0.1882	0.6488	0.4620	2.6397
2457	992.	195.	23.	218.	274.	492.	0.1420	0.2078	0.6456	0.4187	2.7101

SHOCK WAVE PARAMETERS ASSUMING
FROZEN COMPOSITION FOR INCIDENT SHOCKED CONDITIONS

CASE NO. 1207

	CHEMICAL FORMULA	MOLES	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H 2.00000	0.05000	13.478	G	300.00	-0.
FUEL	O 2.00000	0.05000	12.892	G	300.00	-0.
FUEL	AR 1.00000	0.90000	9.191	G	300.00	-0.

O/F= 0. PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.5000 REACTANT DENSITY= 0.

INITIAL GAS (1)									
MACH NO.	3.0480	3.3528	3.6576	3.8100	3.9624	4.1148	4.2672	4.4196	4.5720
U1, M/SEC	1000.00	1100.00	1200.00	1250.00	1300.00	1350.00	1400.00	1450.00	1500.00
P, ATM	0.0132	0.0263	0.0263	0.0263	0.0263	0.0263	0.0263	0.0263	0.0263
T, DEG K	300	300	300	300	300	300	300	300	300
RHO, G/CC	2.0126-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5	4.0253-5
H, CAL/G	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3
S, CAL/(G)(K)	1.2406	1.2041	1.2041	1.2041	1.2041	1.2041	1.2041	1.2041	1.2041
M, MOL WT	37.654	37.654	37.654	37.654	37.654	37.654	37.654	37.654	37.654
CP, CAL/(G)(K)	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372	0.1372
GAMMA (S)	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249	1.6249
SON VEL,M/SEC	328.1	328.1	328.1	328.1	328.1	328.1	328.1	328.1	328.1
SHOCKED GAS (2)--INCIDENT--FROZEN									
U2, M/SEC	317.25	332.77	349.41	358.06	366.89	375.88	385.00	394.24	403.59
P, ATM	0.1488	0.3616	0.4318	0.4692	0.5082	0.5487	0.5908	0.6345	0.6797
T, DEG K	1076	1247	1433	1532	1635	1742	1852	1967	2085
RHO, G/CC	6.3440-5	1.3306-4	1.3824-4	1.4052-4	1.4263-4	1.4457-4	1.4637-4	1.4805-4	1.4961-4
H, CAL/G	107.7	131.5	157.7	171.7	186.1	201.2	216.8	232.9	249.7
S, CAL/(G)(K)	1.2892	1.2629	1.2731	1.2781	1.2830	1.2879	1.2927	1.2974	1.3020
M, MOL WT	37.654	37.654	37.654	37.654	37.654	37.654	37.654	37.654	37.654
CP, CAL/(G)(K)	0.1396	0.1400	0.1404	0.1407	0.1409	0.1411	0.1413	0.1415	0.1418
GAMMA (S)	1.6079	1.6050	1.6020	1.6005	1.5990	1.5975	1.5960	1.5945	1.5930
SON VEL,M/SEC	618.1	664.8	712.1	735.9	759.8	783.8	807.9	832.1	856.3
P2/P1	11.307	13.741	16.409	17.831	19.312	20.852	22.451	24.110	25.827
T2/T1	3.587	4.157	4.778	5.108	5.450	5.806	6.174	6.555	6.949
M2/M1	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
RHO2/RHO1	3.1521	3.3056	3.4343	3.4910	3.5433	3.5916	3.6364	3.6779	3.7167
V2(U1-U2)M/SEC	682.75	767.23	850.59	891.94	933.11	974.12	1015.00	1055.76	1096.41
MOLE FRACTIONS									
H2	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000
O2	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000	0.05000
AR	0.90000	0.90000	0.90000	0.90000	0.90000	0.90000	0.90000	0.90000	0.90000

TRANSPORT PROPERTIES OF THE SHOCKED GAS ASSUMING FROZEN COMPOSITION

O/F= 0. PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.5000 FIRST SHOCK PRESSURE= 0.1488 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	CP FROZ	PRANDTL FROZ
DEG K	POISE	----- CAL/(CM)(SEC)(K) ----			CAL/(G)(K)	
1076	570.X10-6	125.X10-6	14.X10-6	140.X10-6	0.1396	0.5706
1247	630.	139.	17.	155.	0.1400	0.5673
1433	691.	152.	20.	172.	0.1404	0.5641
1532	722.	159.	21.	181.	0.1407	0.5625
1635	754.	166.	23.	189.	0.1409	0.5608
1742	786.	174.	25.	198.	0.1411	0.5591
1852	819.	181.	27.	208.	0.1413	0.5574
1967	852.	188.	29.	217.	0.1415	0.5558
2085	886.	196.	31.	227.	0.1418	0.5542

Case 1565 - Input

```
REACTANTS
N 2.                                 00      .75524          G647.95  0
O 2.                                 00      .23144          G647.95  0
AR1.                                 00      .01286          G647.95  0
C 1.     O 2.                        00      .00046          G647.95  0
C 7.     H 8.                                .4        2867. L 298.15 F
C 8.     H 18.                               .6      -59740. L 298.15 F

NAMELISTS
 $INPT2 KASE=1565, UV=T,V=300,225.24, OF=T,MIX=17,TRACE=1.E-15          $
```

Case 1565 - Output

```
REACTANTS
N    2.0000      -0.          -0.          -0.       00 -0.        0.7552         -0.    G    647.950  0   -0.
O    2.0000      -0.          -0.          -0.       00 -0.        0.2314         -0.    G    647.950  0   -0.
AR   1.0000      -0.          -0.          -0.       00 -0.        0.0129         -0.    G    647.950  0   -0.
C    1.0000  O    2.0000      -0.          -0.       00 -0.        0.0005         -0.    G    647.950  0   -0.
C    7.0000  H    8.0000      -0.          -0.          -0.        0.4000      2867.00  L    298.150  F   -0.
C    8.0000  H   18.0000      -0.          -0.          -0.        0.6000    -59740.00  L    298.150  F   -0.
NAMELISTS

$INPT2

KASE  =            1565,

T     =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,

P     =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

PSIA  =     F, MMHG  =     F, NSQM  =     F,

V     =    3.0000000E+02,    2.2524000E+02,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,

RHO   =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

ERATIO=     F, OF    =     T, FPCT  =     F, FA    =     F,

MIX   =    1.7000000E+01,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,

TP    =     F, HP    =     F, SP    =     F, TV    =     F, UV    =     T, SV    =     F,

RKT   =     F, SHOCK =     F, DETN  =     F, OTTO  =     F, CR    =     0.           , SO    =     0.             , SO    =     0.

IONS  =     F, IDEBUG=                0, TRACE =    1.0000000E-15, SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =     F, PUNCH =     F, NODATA=     F,

$ END

SPECIES BEING CONSIDERED IN THIS SYSTEM
    L 5/66  AR               J 3/61  C(S)             J 3/61  C                J12/67  CH               J 6/69  CH2
    J 3/61  CH2O             J 6/69  CH3              J 3/61  CH4              J 6/69  CN               J 6/66  CNN
    J12/70  CN2              J 9/65  CO               J 9/65  CO2              J12/69  C2               J 3/67  C2H
    J 3/61  C2H2             J 9/65  C2H4             L 5/72  C2H6             J 3/67  C2N              J 3/61  C2N2
    J 9/66  C2O              J12/69  C3               J 6/68  C3O2             J12/69  C4               J12/69  C5
    J 9/65  H                L12/69  HCN              J12/70  HCO              J12/70  HNCO             J 3/63  HNO
    J 3/64  HO2              J 3/61  H2               L11/65  H2O(S)           L11/65  H2O(L)           J 3/61  H2O
    L 2/69  H2O2             J 3/61  N                J12/70  NCO              J12/71  NH               J12/65  NH2
    J 9/65  NH3              J 6/63  NO               J 9/64  NO2              J12/64  NO3              J 9/65  N2
    J12/65  N2H4             J12/64  N2O              J 9/64  N2O4             J12/70  N3               J 6/62  O
    J12/70  OH               J 9/65  O2               J 6/61  O3

OF =  17.000000
                         EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
INTERNAL ENERGY              HPP(2)                   HPP(1)                HSUBO
(KG-MOL)(DEG K)/KG      -0.15164043E+03          0.20365920E+02          0.10810011E+02

KG-ATOMS/KG                 BOP(I,2)                 BOP(I,1)                 BO(I)
       N                0.                       0.53919910E-01          0.50924358E-01
       O                0.                       0.14486447E-01          0.13681644E-01
       AR               0.                       0.32191849E-03          0.30403413E-03
       C                0.72407449E-01           0.10452182E-04          0.40325075E-02
       H                0.12927296E+00           0.                      0.71818314E-02

PT       N        O        AR        C        H
 1   -12.574  -15.095  -23.385  -19.796  -11.805   14.000
 2   -12.386  -14.965  -23.104  -19.710  -11.711    3.000
```

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

VOLUME

CASE NO. 1565

CHEMICAL FORMULA					WT FRACTION (SEE NOTE)	ENERGY \CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT N	2.00000				0.75524	1184.555	G	647.95	-0.
OXIDANT O	2.00000				0.23144	1292.515	G	647.95	-0.
OXIDANT AR	1.00000				0.01286	450.192	G	647.95	-0.
OXIDANT C	1.00000	O	2.00000		0.00046	-91701.919	G	647.95	-0.
FUEL C	7.00000	H	8.00000		0.40000	2867.000	L	298.15	-0.
FUEL C	8.00000	H	18.00000		0.60000	-59740.000	L	298.15	-0.

O/F= 17.0000 PERCENT FUEL= 5.5556 EQUIVALENCE RATIO= 0.8519 REACTANT DENSITY= 0.

THERMODYNAMIC PROPERTIES

U, CAL/G	21.48	21.48
P, ATM	25.578	34.181
T, DEG K	2693	2704
RHO, G/CC	3.3333-3	4.4397-3
H, CAL/G	207.3	207.9
S, CAL/(G)(K)	2.0960	2.0762
M, MOL WT	28.800	28.820
(DLV/DLP)T	-1.00380	-1.00353
(DLV/DLT)P	1.0946	1.0876
CP, CAL/(G)(K)	0.5164	0.5040
GAMMA (S)	1.1852	1.1881
SON VEL,M/SEC	960.0	962.7

MOLE FRACTIONS

AR	8.7562-3	8.7623-3
C	6.404-15	5.993-15
CH	1.158-15	1.172-15
CH2O	2.843-10	3.212-10
CH3	3.222-15	3.679-15
CN	7.571-12	7.784-12
CN2	2.283-15	2.739-15
CO	1.1627-2	1.0745-2
CO2	1.0451-1	1.0547-1
C2O	1.155-15	1.262-15
H	4.4450-4	3.8337-4
HCN	3.005-10	3.241-10
HCO	1.4378-8	1.5108-8
HNCO	2.6951-9	3.1952-9
HNO	1.0667-6	1.1919-6
HO2	6.3652-6	6.9525-6
H2	1.6653-3	1.5251-3
H2O	9.8202-2	9.8591-2
H2O2	9.1393-7	1.0745-6
N	2.5831-7	2.4367-7
NCO	3.186-10	3.581-10
NH	1.8630-8	1.9082-8
NH2	3.2741-8	3.5684-8
NH3	1.3017-8	1.5106-8
NO	1.1523-2	1.1624-2
NO2	1.4118-5	1.6171-5
NO3	8.310-11	1.102-10
N2	7.2754-1	7.2800-1
N2O	2.8153-6	3.2851-6
N3	3.821-11	4.774-11
O	1.1500-3	1.0335-3
OH	6.6493-3	6.3554-3
O2	2.7908-2	2.7480-2
O3	1.1540-8	1.3380-8

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.10000E-14 FOR ALL ASSIGNED CONDITIONS

C(S)	CH2	CH4	CNN	C2	C2H	C2H2	C2H4	C2H6	C2N
C2N2	C3	C3O2	C4	C5	H2O(S)	H2O(L)	N2H4	N2O4	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

NO TRANSPORT DATA WAS FOUND FOR THE SPECIES HO2

TRANSPORT PROPERTIES AT ASSIGNED VOLUME

O/F= 17.0000 PERCENT FUEL= 5.5556 EQUIVALENCE RATIO= 0.8519 INTERNAL ENERGY= 21.48 CAL/G

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	---------- CAL/(CM)(SEC)(K) ----------					CAL/(G)(K)		---- DIMENSIONLESS -----		
2693	818.X10-6	215.X10-6	189.X10-6	404.X10-6	270.X10-6	674.X10-6	0.3413	0.5164	0.6913	0.6265	1.3049

NO TRANSPORT DATA WAS FOUND FOR THE SPECIES HO2

2704	821.	215.	190.	405.	250.	655.	0.3414	0.5040	0.6915	0.6317	1.2930

Case 5612 - Input

```
REACTANTS
N 2.     H 4.                                  80.    12050.   L298.15  F 1.0036
BE1.                                           20.    0.0      S298.15  F 1.85
H 2.     O 2.                                  100.   -44880.  L298.15  O 1.407

INSERT          BEO(L)
NAMELISTS
 $INPT2  KASE=5612,FPCT=T, MIX=67, P=1000,500,PSIA=T, RKT=T, NODATA=T $
 $RKTINP  PCP=3,10,30,300,  FROZ=F                                     $
```

Case 5612 - Output

```
REACTANTS
N   2.0000  H    4.0000      -0.          -0.          -0.        80.0000      12050.00  L   298.150  F    1.00360
BE  1.0000      -0.          -0.          -0.          -0.        20.0000          0.    S   298.150  F    1.85000
H   2.0000  O    2.0000      -0.          -0.          -0.       100.0000     -44880.00  L   298.150  O    1.40700
INSERT          BEO(L)
NAMELISTS

$INPT2

KASE  =              5612,

T     =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,

P     =    1.0000000E+03,    5.0000000E+02,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

PSIA  =     T, MMHG  =     F, NSQM  =     F,

V     =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,

RHO   =    1.0000000E+03,    5.0000000E+02,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,

ERATIO=     F, OF    =     F, FPCT  =     T, FA    =     F,

MIX   =    6.7000000E+01,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,

TP    =     F, HP    =     F, SP    =     F, TV    =     F, UV    =     F, SV    =     F,

RKT   =     T, SHOCK =     F, DETN  =     F, OTTO  =     F, CR    =    0.           , SO    =    0.           , SO    =    0.

IONS  =     F, IDEBUG=                0, TRACE =    0.           , SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =     F, PUNCH =     F, NODATA=     T,

$ END

SPECIES BEING CONSIDERED IN THIS SYSTEM
    J 9/61  BE(S)          J 9/61  BE(L)          J 9/61  BE             J 3/63  BEH            J 6/63  BEN
    J 6/71  BEO(S)         J 6/71  BEO(S)         J 6/71  BEO(L)         J 9/63  BEO            J 9/63  BEOH
    J 3/67  BEO2H2         J 9/63  BE2O           J 9/63  BE2O2          J 9/63  BE3O3          J 9/63  BE4O4
    J 9/65  H              J 3/63  HNO            J 3/64  HO2            J 3/61  H2             L11/65  H2O(S)
    L11/65  H2O(L)         J 3/61  H2O            L 2/69  H2O2           J 3/61  N              J12/71  NH
    J12/65  NH2            J 9/65  NH3            J 6/63  NO             J 9/64  NO2            J12/64  NO3
    J 9/65  N2             J12/65  N2H4           J12/64  N2O            J 9/64  N2O4           J12/70  N3
    J 6/62  O              J12/70  OH             J 9/65  O2             J 6/61  O3

$RKTINP

EQL   =     T, FROZ  =     F,

SUBAR =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,

SUPAR =    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
           0.           ,    0.           ,    0.           ,    0.           ,    0.           ,    0.           ,
                        ,
```

```
PCP    =   3.0000000E+00,    1.0000000E+01,    3.0000000E+01,    3.0000000E+02,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

NFZ    =                1,

$ END

OF =  0.492537
                          EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                        HPP(2)                  HPP(1)                HSUBO
(KG-MOL)(DEG K)/KG        0.15138364E+03          -0.66397491E+03       -0.11768468E+03

KG-ATOMS/KG                   BOP(I,2)                BOP(I,1)              BO(I)
       N                  0.49929349E-01          0.                    0.33452664E-01
       H                  0.99858698E-01          0.58798038E-01        0.86308680E-01
       BE                 0.22192139E-01          0.                    0.14868733E-01
       O                  0.                      0.58798038E-01        0.19403352E-01

PT      N         H         BE        O
 1  -12.759   -8.578  -13.145  -20.218   11.000
 2  -12.897   -8.719  -13.764  -20.839    3.000
PC/PT= 1.748578   T =  2844.77
 2  -12.897   -8.720  -13.766  -20.841    2.000
PC/PT= 1.751558   T =  2844.13
 3  -13.027   -8.855  -14.461  -21.526    3.000
 3  -13.084   -8.910  -14.166  -21.236    3.000
 4  -13.688   -9.517  -14.169  -21.233    3.000
 4  -13.476   -9.311  -15.668  -22.379    4.000
 5  -13.730   -9.579  -18.318  -24.378    4.000
 5  -13.752   -9.600  -18.141  -24.210    3.000
 6  -14.276  -10.158  -26.901  -30.508    4.000

                THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC =  1000.0 PSIA
CASE NO.    5612

        CHEMICAL FORMULA                                          WT FRACTION   ENERGY   STATE   TEMP     DENSITY
                                                                  (SEE NOTE)    CAL/MOL          DEG K    G/CC
FUEL    N  2.00000   H  4.00000                                    0.80000    12050.000   L    298.15   1.0036
FUEL    BE 1.00000                                                0.20000        0.       S    298.15   1.8500
OXIDANT H  2.00000   O  2.00000                                    1.00000   -44880.000   L    298.15   1.4070

              O/F=  0.4925     PERCENT FUEL= 67.0000     EQUIVALENCE RATIO=  2.9904     REACTANT DENSITY=  1.1890

                CHAMBER    THROAT      EXIT       EXIT       EXIT       EXIT
PC/P              1.0000    1.7516    3.0000    10.000     30.000     300.00
P, ATM           68.046    38.849    22.682     6.8046     2.2682     0.2268
T, DEG K           3068      2844      2721       2423       2071       1402
RHO, G/CC     4.4700-3  2.7624-3  1.6878-3  5.7008-4  2.2271-4  3.2936-5
H, CAL/G         -233.9    -432.6    -610.0     -987.1    -1282.2    -1753.7
S, CAL/(G)(K)     3.4110    3.4110    3.4110     3.4110     3.4110     3.4110

M, MOL WT         16.536    16.595    16.612     16.654     16.688     16.700
(DLV/DLP)T       -1.00511  -1.00328  -1.00273   -1.00141   -1.00036   -1.00001
(DLV/DLT)P        1.0924    1.0633    0.         1.0317     1.0093     1.0001
CP, CAL/(G)(K)    0.9894    0.9257    0.         0.8341     0.7515     0.6703
GAMMA (S)         1.1625    1.1668    0.9973     1.1777     1.1920     1.2159
SON VEL,M/SEC     1339.1    1289.4    1165.3     1193.5     1109.1     921.1
MACH NUMBER       0.        1.000     1.522      2.104      2.671      3.872

AE/AT                       1.0000    1.1895     2.4888     5.4000     30.326
CSTAR, FT/SEC                6351      6351       6351       6351       6351
CF                          0.666     0.917      1.297      1.530      1.842
IVAC,LB-SEC/LB              244.2     259.2      305.1      337.6      383.6
ISP, LB-SEC/LB              131.5     180.9      256.0      302.0      363.6


MOLE FRACTIONS

BE                0.00003   0.00001   0.00000   0.00000   0.        0.
BEH               0.00001   0.00000   0.00000   0.00000   0.        0.
BEO(S)            0.        0.        0.        0.        0.19872   0.19891
BEO(S)            0.        0.        0.07071   0.19809   0.        0.
BEO(L)            0.19539   0.19660   0.12632   0.        0.        0.
BEOH              0.00032   0.00013   0.00008   0.00001   0.00000   0.
BEO2H2            0.00207   0.00149   0.00120   0.00047   0.00010   0.00000
H                 0.01490   0.00974   0.00821   0.00433   0.00111   0.00001
H2                0.50639   0.51002   0.51105   0.51362   0.51586   0.51665
H2O               0.05765   0.05863   0.05902   0.05999   0.06052   0.06066
NH2               0.00002   0.00001   0.00001   0.00000   0.00000   0.
NH3               0.00010   0.00006   0.00004   0.00002   0.00001   0.00000
NO                0.00004   0.00002   0.00001   0.00000   0.00000   0.
N2                0.22247   0.22295   0.22307   0.22337   0.22366   0.22376
O                 0.00001   0.00000   0.00000   0.00000   0.00000   0.
OH                0.00060   0.00033   0.00025   0.00009   0.00001   0.00000

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.50000E-05 FOR ALL ASSIGNED CONDITIONS

BE(S)       BE(L)       BEN         BEO         BE2O        BE2O2       BE3O3       BE4O4       HNO         HO2
H2O(S)      H2O(L)      H2O2        N           NH          NO2         NO3         N2H4        N2O         N2O4
N3          O2          O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS
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TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

O/F= 0.4925 PERCENT FUEL= 67.0000 EQUIVALENCE RATIO= 2.9904 CHAMBER PRESSURE= 68.046 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		---- DIMENSIONLESS -----		
3068	688.X10-6	766.X10-6	673.X10-6	1439.X10-6	1165.X10-6	2603.X10-6	0.8782	1.1951	0.4200	0.3159	2.2428
2844	651.	718.	620.	1338.	823.	2161.	0.8691	1.1033	0.4224	0.3321	2.2818
2721	630.	694.	590.	1284.	727.	2010.	0.8634	1.0763	0.4236	0.3371	2.2963
2423	579.	634.	516.	1150.	433.	1583.	0.8478	0.9850	0.4266	0.3601	2.3260
2071	518.	564.	428.	993.	131.	1123.	0.8251	0.8716	0.4304	0.4018	2.3350
1402	397.	434.	266.	700.	1.	702.	0.7677	0.7683	0.4348	0.4344	2.2061

PT	N	H	BE	O	
1	-13.091	-8.912	-13.214	-20.295	3.000
2	-13.233	-9.057	-13.817	-20.889	3.000
PC/PT= 1.745202 T = 2828.07					
2	-13.233	-9.058	-13.819	-20.891	2.000
PC/PT= 1.749179 T = 2827.43					
3	-13.368	-9.196	-14.499	-21.562	3.000
3	-13.432	-9.259	-14.167	-21.235	3.000
4	-14.037	-9.869	-14.171	-21.230	3.000
4	-13.818	-9.654	-15.709	-22.408	4.000
5	-14.077	-9.926	-18.316	-24.376	4.000
5	-14.099	-9.947	-18.142	-24.210	3.000
6	-14.624	-10.506	-26.862	-30.481	4.000

THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 500.0 PSIA
CASE NO. 5612

CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000	H 4.00000		0.80000	12050.000	L	298.15	1.0036
FUEL	BE 1.00000			0.20000	0.	S	298.15	1.8500
OXIDANT	H 2.00000	O 2.00000		1.00000	-44880.000	L	298.15	1.4070

O/F= 0.4925 PERCENT FUEL= 67.0000 EQUIVALENCE RATIO= 2.9904 REACTANT DENSITY= 1.1890

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7492	3.0000	10.000	30.000	300.00
P, ATM	34.023	19.451	11.341	3.4023	1.1341	0.1134
T, DEG K	3041	2827	2721	2416	2071	1404
RHO, G/CC	2.2475-3	1.3882-3	8.4200-4	2.8556-4	1.1133-4	1.6445-5
H, CAL/G	-233.9	-431.1	-608.9	-985.4	-1280.4	-1752.3
S, CAL/(G)(K)	3.4945	3.4945	3.4945	3.4945	3.4945	3.4945
M, MOL WT	16.485	16.559	16.575	16.637	16.683	16.700
(DLV/DLP)T	-1.00656	-1.00430	-1.00380	-1.00191	-1.00050	-1.00001
(DLV/DLT)P	1.1213	1.0846	0.	1.0435	1.0131	1.0001
CP, CAL/(G)(K)	1.0570	0.9780	0.	0.8663	0.7636	0.6707
GAMMA (S)	1.1585	1.1629	0.9962	1.1740	1.1899	1.2158
SON VEL,M/SEC	1333.0	1284.9	1166.0	1190.5	1108.3	921.7
MACH NUMBER	0.	1.000	1.519	2.107	2.670	3.867
AE/AT		1.0000	1.1958	2.4908	5.4142	30.428
CSTAR, FT/SEC		6341	6341	6341	6341	6341
CF		0.665	0.917	1.298	1.531	1.844
IVAC,LB-SEC/LB		243.7	259.2	304.8	337.3	383.5
ISP, LB-SEC/LB		131.0	180.6	255.7	301.8	363.5

MOLE FRACTIONS

BE	0.00005	0.00001	0.00001	0.00000	0.00000	0.
BEH	0.00001	0.00000	0.00000	0.00000	0.	0.
BEO(S)	0.	0.	0.	0.	0.19868	0.19891
BEO(S)	0.	0.	0.08351	0.19793	0.	0.
BEO(L)	0.19488	0.19626	0.11314	0.	0.	0.
BEOH	0.00040	0.00016	0.00011	0.00002	0.00000	0.
BEO2H2	0.00198	0.00144	0.00120	0.00046	0.00010	0.00000
H	0.01942	0.01297	0.01159	0.00592	0.00156	0.00001
H2	0.50298	0.50760	0.50853	0.51242	0.51552	0.51665
H2O	0.05742	0.05846	0.05882	0.05992	0.06050	0.06066
NH2	0.00002	0.00001	0.00000	0.00000	0.00000	0.
NH3	0.00005	0.00003	0.00002	0.00001	0.00000	0.00000
NO	0.00006	0.00003	0.00002	0.00001	0.00000	0.
N2	0.22194	0.22258	0.22269	0.22319	0.22361	0.22376
O	0.00002	0.00001	0.00001	0.00000	0.00000	0.
OH	0.00076	0.00043	0.00035	0.00013	0.00002	0.00000

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

BE(S)	BE(L)	BEN	BED	BE2O	BE2O2	BE3O3	BE4O4	HNO	HO2
H2O(S)	H2O(L)	H2O2	N	NH	NO2	NO3	N2H4	N2O	N2O4
N3	O2	O3							

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

O/F= 0.4925 PERCENT FUEL= 67.0000 EQUIVALENCE RATIO= 2.9904 CHAMBER PRESSURE= 34.023 ATM

TEMP	VISCOSITY	MONAIDMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	---------- CAL/(CM)(SEC)(K) ----------					CAL/(G)(K)		---- DIMENSIONLESS -----		
3041	534.X10-6	768.X10-6	663.X10-6	1432.X10-6	1529.X10-6	2961.X10-6	0.8773	1.2974	0.4193	0.2999	2.2294
2827	648.	720.	614.	1334.	1101.	2436.	0.8685	1.1841	0.4219	0.3151	2.2717
2721	630.	698.	588.	1287.	1024.	2311.	0.8636	1.1646	0.4229	0.3175	2.2842
2416	578.	634.	514.	1148.	593.	1742.	0.8476	1.0363	0.4263	0.3437	2.3208
2071	518.	565.	428.	993.	185.	1178.	0.8251	0.8908	0.4303	0.3918	2.3341
1404	397.	434.	267.	701.	2.	703.	0.7679	0.7688	0.4348	0.4342	2.2476

Case 6666 - Input

```
REACTANTS
H 2.                                    100.    -2154.   L 20.27  F .0709
O 2.                                    100.    -3102.   L90.18   O 1.149

NAMELIST
 $INPT2 KASE=6666, P=3000, PSIA=T, FPCT=T, MIX=20, RKT=T                $
 $RKTINP SUPAR=1.5,2.5,4., PCP=2.5,3,4,10,30, SUBAR=2,3,10, NFZ=4,  $
```

Case 6666 - Output

```
REACTANTS
H   2.0000    -0.         -0.         -0.         -0.      100.0000      -2154.00  L    20.270  F    0.07090
O   2.0000    -0.         -0.         -0.         -0.      100.0000      -3102.00  L    90.180  O    1.14900
NAMELIST

$INPT2

KASE  =              6666,

T     =    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

P     =    3.0000000E+03,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,

PSIA  =     T, MMHG  =     F, NSQM  =     F,

V     =    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,

RHO   =    3.0000000E+03,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,

ERATIO=     F, OF    =     F, FPCT  =     T, FA    =     F,

MIX   =    2.0000000E+01,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

IP    =     F, HP    =     F, SP    =     F, TV    =     F, UV    =     F, SV    =     F,

RKT   =     T, SHOCK =     F, DETN  =     F, OTTO  =     F, CR    =    0.          , SO    =    0.          , SO    =    0.

IONS  =     F, IDEBUG=              0, TRACE =    0.          , SIUNIT=     F, EUNITS=     F,

TRNSPT=     T, FROZN =     F, PUNCH =     F, NODATA=     F,

$ END

SPECIES BEING CONSIDERED IN THIS SYSTEM
    J 9/65  H                J 3/64  HO2              J 3/61  H2               L11/65  H2O(S)           L11/65  H2O(L)
    J 3/61  H2O              L 2/69  H2O2             J 6/62  O                J12/70  OH               J 9/65  O2
    J 6/61  O3

$RKTINP

EQL   =     T, FROZ  =     T,

SUBAR =    2.0000000E+00,    3.0000000E+00,    1.0000000E+01,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,

SUPAR =    1.5000000E+00,    2.5000000E+00,    4.0000000E+00,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,

PCP   =    2.5000000E+00,    3.0000000E+00,    4.0000000E+00,    1.0000000E+01,    3.0000000E+01,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,    0.          ,    0.          ,
           0.          ,    0.          ,    0.          ,    0.          ,

NFZ   =              4,

$ END
```

```
OF =   4.000000
                                EFFECTIVE FUEL          EFFECTIVE OXIDANT          MIXTURE
ENTHALPY                            HPP(2)                  HPP(1)                 HSUBO
(KG-MOL)(DEG K)/KG          -0.53769263E+03         -0.48783627E+02         -0.14656543E+03

KG-ATOMS/KG                       BOP(I,2)                BOP(I,1)                BO(I)
      H                       0.99209300E+00          0.                      0.19841859E+00
      O                       0.              0.62502343E-01          0.50001875E-01

PT      H          U
 1    -8.106   -18.242    9.000
 2    -8.224   -19.064    3.000
PC/PT= 1.770715    T =  2719.66
 2    -8.225   -19.070    2.000
PC/PT= 1.777559    T =  2717.89
 2    -8.225   -19.070    1.000
PC/PT= 1.777525    T =  2717.86
 3    -8.293   -19.634    3.000
 4    -8.329   -19.961    3.000
 5    -8.386   -20.513    3.000
 6    -8.563   -22.618    3.000
 7    -8.774   -25.980    3.000
 8    -8.116   -18.305    8.000
 8    -8.118   -18.318    2.000
 8    -8.118   -18.320    2.000
 8    -8.118   -18.320    1.000
 9    -8.110   -18.270    2.000
 9    -8.111   -18.274    2.000
 9    -8.111   -18.275    1.000
10    -8.106   -18.247    2.000
10    -8.106   -18.244    2.000
10    -8.105   -18.245    1.000
10    -8.106   -18.245    1.000
10    -8.106   -18.245    1.000
11    -8.438   -21.072    4.000
11    -8.439   -21.083    2.000
12    -8.599   -23.125    3.000
12    -8.601   -23.148    1.000
13    -8.742   -25.405    3.000
13    -8.736   -25.300    1.000

                THEORETICAL ROCKET PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC =  3000.0 PSIA
CASE NO.    6666

                                                                  WT FRACTION   ENERGY   STATE   TEMP    DENSITY
        CHEMICAL FORMULA                                          (SEE NOTE)   CAL/MOL          DEG K   G/CC
FUEL    H  2.00000                                                  1.00000    -2154.000   L     20.27   0.0709
OXIDANT O  2.00000                                                  1.00000    -3102.000   L     90.18   1.1490

          O/F=  4.0000    PERCENT FUEL= 20.0000    EQUIVALENCE RATIO=  1.9841    REACTANT DENSITY=  0.2843

                  CHAMBER   THROAT    EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT      EXIT
PC/P                1.0000    1.7776    2.5000    3.0000    4.0000   10.000    30.000    1.0601    1.0247    1.0021    5.2560   12.183    24.655
P, ATM             204.14    114.84     81.655    68.046    51.034    20.414    6.8046   192.56    199.21    203.71    38.839   16.756     8.2797
T, DEG K             2988      2718      2563      2482      2357      1984      1593      2960      2977      2987      2241     1909      1658
RHO, G/CC       8.3498-3  5.1773-3  3.9076-3  3.3640-3  2.6581-3  1.2639-3  5.2480-4  7.9531-3  8.1813-3  8.3351-3  2.1276-3  1.0781-3  6.1339-4
H, CAL/G           -291.2    -615.9    -793.8    -884.6   -1021.9   -1413.5   -1799.7    -325.6    -305.7    -292.5   -1145.7   -1489.2   -1736.8
S, CAL/(G)(K)       4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111    4.9111

M, MOL WT          10.029    10.054    10.064    10.068    10.072    10.078    10.080    10.032    10.031    10.029    10.075    10.079    10.080
(DLV/DLP)T      -1.00251  -1.00126  -1.00078  -1.00059  -1.00037  -1.00006  -1.00000  -1.00236  -1.00245  -1.00251  -1.00023  -1.00004  -1.00001
(DLV/DLT)P          1.0495    1.0270    1.0176    1.0138    1.0090    1.0017    1.0001    1.0468    1.0484    1.0494    1.0058    1.0011    1.0002
CP, CAL/(G)(K)      1.2974    1.1978    1.1491    1.1263    1.0945    1.0199    0.9569    1.2864    1.2928    1.2970    1.0686    1.0074    0.9674
GAMMA (S)           1.1986    1.2088    1.2153    1.2188    1.2242    1.2406    1.2595    1.1996    1.1990    1.1987    1.2293    1.2440    1.2561
SON VEL,M/SEC       1723.1    1648.3    1604.1    1580.5    1543.2    1424.9    1286.4    1715.5    1719.9    1722.9    1507.9    1399.6    1310.7
MACH NUMBER             0.     1.000     1.278     1.410     1.602     2.151     2.762     0.313     0.202     0.060     1.773     2.262     2.654

AE/AT                           1.0000    1.0650    1.1385    1.2984    2.2034    4.5769    2.0000    3.0000    10.000    1.5000    2.5000    4.0000
CSTAR, FT/SEC                    7952      7952      7952      7952      7952      7952      7952      7952      7952      7952      7952      7952
CF                              0.680     0.846     0.919     1.020     1.264     1.466     0.221     0.143     0.042     1.103     1.306     1.435
IVAC,LB-SEC/LB                  307.1     314.4     321.0     332.4     366.9     400.0     521.0     759.0    2466.9     343.2     373.6     394.8
ISP, LB-SEC/LB                  168.1     209.1     227.2     252.1     312.5     362.3      54.7      35.5      10.5     272.7     322.9     354.7


MOLE FRACTIONS

H                   0.00743   0.00396   0.00255   0.00197   0.00126   0.00023   0.00001   0.00701   0.00725   0.00741   0.00080   0.00015   0.00002
H2                  0.49109   0.49340   0.49424   0.49463   0.49511   0.49583   0.49599   0.49135   0.49120   0.49110   0.49543   0.49589   0.49598
H2O                 0.49895   0.50168   0.50264   0.50300   0.50341   0.50392   0.50400   0.49930   0.49910   0.49896   0.50365   0.50395   0.50400
O                   0.00002   0.00001   0.00000   0.00000   0.00000   0.        0.        0.00002   0.00002   0.00002   0.00000   0.        0.
OH                  0.00249   0.00105   0.00057   0.00040   0.00022   0.00002   0.00000   0.00230   0.00241   0.00248   0.00012   0.00001   0.00000
O2                  0.00001   0.00000   0.00000   0.00000   0.00000   0.        0.        0.00001   0.00001   0.00001   0.00000   0.        0.

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN  0.50000E-05 FOR ALL ASSIGNED CONDITIONS

HO2          H2O(S)       H2O(L)       H2O2         O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS
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TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

O/F= 4.0000 PERCENT FUEL= 20.0000 EQUIVALENCE RATIO= 1.9841 CHAMBER PRESSURE= 204.137 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	REACTION COND	EQUILIBRIUM COND	CP FROZ	CP EQ	PRANDTL FROZ	PRANDTL EQ	LEWIS NUMBER
DEG K	POISE	CAL/(CM)(SEC)(K)					CAL/(G)(K)		DIMENSIONLESS		
2988	854.X10-6	790.X10-6	892.X10-6	1682.X10-6	542.X10-6	2224.X10-6	1.1019	1.2974	0.5596	0.4982	1.8171
2718	796.	734.	803.	1537.	311.	1848.	1.0826	1.1978	0.5605	0.5158	1.9025
2563	761.	702.	751.	1453.	210.	1662.	1.0700	1.1491	0.5607	0.5262	1.9517
2482	743.	685.	723.	1408.	166.	1574.	1.0629	1.1263	0.5607	0.5314	1.9773
2357	714.	660.	679.	1339.	111.	1450.	1.0511	1.0945	0.5606	0.5389	2.0162
1984	624.	582.	946.	1128.	23.	1152.	1.0102	1.0199	0.5590	0.5530	2.1195
1593	524.	498.	409.	907.	2.	909.	0.9561	0.9569	0.5525	0.5520	2.1732
2960	848.	784.	883.	1667.	515.	2182.	1.1001	1.2864	0.5597	0.4999	1.8258
2977	852.	787.	888.	1675.	531.	2206.	1.1012	1.2928	0.5596	0.4990	1.8207
2987	854.	790.	892.	1681.	541.	2222.	1.1019	1.2970	0.5596	0.4983	1.8174
2241	687.	536.	638.	1274.	73.	1347.	1.0394	1.0686	0.5604	0.5448	2.0512
1909	605.	566.	520.	1086.	15.	1102.	1.0008	1.0074	0.5581	0.5540	2.1350
1658	542.	513.	432.	944.	3.	947.	0.9660	0.9674	0.5540	0.5531	2.1696

THEORETICAL ROCKET PERFORMANCE ASSUMING FROZEN COMPOSITION DURING EXPANSION AFTER POINT 4

PC = 3000.0 PSIA
CASE NO. 6666

	CHEMICAL FORMULA	WT FRACTION (SEE NOTE)	ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	H 2.00000	1.00000	-2154.000	L	20.27	0.0709
OXIDANT	O 2.00000	1.00000	-3102.000	L	90.18	1.1490

O/F= 4.0000 PERCENT FUEL= 20.0000 EQUIVALENCE RATIO= 1.9841 REACTANT DENSITY= 0.2843

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.0000	1.7776	2.5000	3.0000	4.0000	10.000	30.000	5.2795	12.257	24.810
P, ATM	204.14	114.84	81.655	68.046	51.034	20.414	6.8046	38.666	16.655	8.2280
T, DEG K	2988	2718	2563	2482	2352	1973	1582	2232	1896	1645
RHO, G/CC	8.3498-3	5.1773-3	3.9076-3	3.3640-3	2.6622-3	1.2693-3	5.2765-4	2.1256-3	1.0778-3	6.1357-4
H, CAL/G	-291.2	-615.9	-793.8	-884.6	-1021.8	-1412.1	-1796.5	-1147.3	-1489.8	-1736.0
S, CAL/(G)(K)	4.9111	4.9111	4.9111	4.9111	4.9111	4.9111	4.9111	4.9111	4.9111	4.9111
M, MOL WT	10.029	10.054	10.064	10.068	10.068	10.068	10.068	10.068	10.068	10.068
CP, CAL/(G)(K)	1.2974	1.1978	1.1491	1.1263	1.0507	1.0090	0.9547	1.0385	0.9993	0.9643
GAMMA (S)	1.1986	1.2088	1.2153	1.2188	1.2313	1.2432	1.2606	1.2347	1.2461	1.2573
SON VEL,M/SEC	1723.1	1648.3	1604.1	1580.5	1546.5	1423.3	1283.4	1508.5	1396.8	1307.1
MACH NUMBER	0.	1.000	1.278	1.410	1.599	2.152	2.765	1.774	2.267	2.660
AE/AT		1.0000	1.0650	1.1385	1.2965	2.1953	4.5571	1.5000	2.5000	4.0000
CSTAR, FT/SEC		7952	7952	7952	7952	7952	7952	7952	7952	7952
CF		0.680	0.846	0.919	1.020	1.264	1.464	1.104	1.307	1.434
IVAC,LB-SEC/LB		307.1	314.4	321.0	332.2	366.6	399.4	343.1	373.4	394.4
ISP, LB-SEC/LB		168.1	209.1	227.2	252.1	312.3	361.9	272.9	322.9	354.6

MOLE FRACTIONS

H	0.00197	H2	0.49463	H2O	0.50300	OH	0.00040

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-05 FOR ALL ASSIGNED CONDITIONS

HO2 H2O(S) H2O(L) H2O2 O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

TRANSPORT PROPERTIES OF ROCKET EXHAUST ASSUMING FROZEN COMPOSITION DURING EXPANSION FROZEN AFTER POINT 4

O/F= 4.0000 PERCENT FUEL= 20.0000 EQUIVALENCE RATIO= 1.9841 CHAMBER PRESSURE= 204.137 ATM

TEMP	VISCOSITY	MONATOMIC COND	INTERNAL COND	FROZEN COND	CP FROZ	PRANDTL FROZ
DEG K	POISE	CAL/(CM)(SEC)(K)			CAL/(G)(K)	
2988	854.X10-6	790.X10-6	892.X10-6	1682.X10-6	1.1019	0.5596
2718	796.	734.	803.	1537.	1.0826	0.5605
2563	761.	702.	751.	1453.	1.0700	0.5607
2482	743.	685.	723.	1408.	1.0629	0.5607
2352	713.	659.	677.	1336.	1.0507	0.5605
1973	622.	581.	542.	1123.	1.0090	0.5585
1582	521.	497.	405.	902.	0.9547	0.5519
2232	684.	635.	634.	1269.	1.0385	0.5601
1896	602.	565.	515.	1080.	0.9993	0.5576
1645	538.	511.	427.	938.	0.9643	0.5533

REFERENCES

1. Gordon, Sanford; and McBride, Bonnie J.: Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouguet Detonations. NASA SP-273, 1971.

2. Zeleznik, Frank J.; and Gordon, Sanford: Calculation of Complex Chemical Equilibria. Ind. Eng. Chem., vol. 60, no. 6, June 1968, pp. 27-57.

3. Zeleznik, Frank J.; and Gordon, Sanford: An Analytical Investigation of Three General Methods of Calculating Chemical-Equilibrium Compositions. NASA TN D-473, 1960.

4. Van Zeggeren, F.; and Storey, S. H.: The Computation of Chemical Equilibria. Cambridge Univ. Press, 1970.

5. Beirute, Roberto M.; and Henley, Ernest J.: A Thermodynamics and Physical Properties Package. Dept. of Chem. Eng., Cullen College of Eng., Univ. of Houston, Jan. 1969.

6. Croom, Bobby H.; and Leyhe, Edward W.: Thermodynamic, Transport, and Flow Properties for the Products of Methane Burned in Oxygen-Enriched Air. NASA SP-3035, 1966.

7. Taylor, M. V.; and Petrozzi, P. J.: A Practical Computer Program for the Calculation of Transport Properties of Gases. Tech. Paper 2 LRO, Aerojet-General Corp., Aug. 17, 1964.

8. Yos, Jerrold M.: Transport Properties of Nitrogen, Hydrogen, Oxygen, and Air to 30,000° K. Rep. RAD-TM-63-7, Avco Corp., Mar. 22, 1963.

9. Rigdon, W. S.: A Computer Code for Calculation of Transport Properties of High-Temperature Gases. Rep. DAC-59134, Douglas Aircraft Co., Inc., July 1968.

10. Devoto, R. S.: Transport Properties of Ionized Monatomic Gases. Phys. Fluids, vol. 9, no. 6, June 1966, pp. 1230-1240.

11. Devoto, R. S.: Transport Coefficients of Partially Ionized Argon. Phys. Fluids, vol. 10, no. 2, Feb. 1967, pp. 354-364.

12. McBride, Bonnie J.; and Gordon, Sanford: FORTRAN IV Program for Calculation of Thermodynamic Data. NASA TN D-4097, 1967.

13. Chapman, Sydney; and Cowling, T. G.: The Mathematical Theory of Non-Uniform Gases. Second ed., Cambridge Univ. Press, 1952.

14. Hirschfelder, Joseph O.; Curtiss, Charles F.; and Bird, R. Byron: Molecular Theory of Gases and Liquids. John Wiley & Sons, Inc., 1954.

15. Grad, Harold: On the Kinetic Theory of Rarefied Gases. Comm. Pure Appl. Math., vol. 2, no. 4, Dec. 1949, pp. 331-407.

16. Muckenfuss, Charles; and Curtiss, C. F.: Thermal Conductivity of Multicomponent Gas Mixtures. J. Chem. Phys., vol. 29, no. 6, Dec. 1958, pp. 1273-1277.

17. Monchick, L.; Yun, K. S.; and Mason, E. A.: Formal Kinetic Theory of Transport Phenomena in Polyatomic Gas Mixtures. J. Chem. Phys., vol. 39, no. 3, Aug. 1, 1963, pp. 654-669.

18. Monchick, L.; Pereira, A. N. G.; and Mason, E. A.: Heat Conductivity of Polyatomic and Polar Gases and Gas Mixtures. J. Chem. Phys., vol. 42, no. 9, May 1, 1965, pp. 3241-3256.

19. Hirschfelder, Joseph O.: Generalization of the Eucken Approximation for the Heat Conductivity of Polyatomic or Chemically Reacting Gas Mixtures. Proceedings of the Conference on Thermodynamic and Transport Properties of Fluids. Inst. Mech. Eng. and Int. Union of Pure and Appl. Chem., 1958, pp. 133-141.

20. Mason, E. A.; and Monchick, L.: Heat Conductivity of Polyatomic and Polar Gases. J. Chem. Phys., vol. 36, no. 6, Mar. 15, 1962, pp. 1622-1639.

21. Butler, James N.; and Brokaw, Richard S.: Thermal Conductivity of Gas Mixtures in Chemical Equilibrium. J. Chem. Phys., vol. 26, no. 6, June 1957, pp. 1636-1643.

22. Brokaw, Richard S.: Thermal Conductivity of Gas Mixtures in Chemical Equilibrium. II. J. Chem. Phys., vol. 32, no. 4, Apr. 1960, pp. 1005-1006.

23. Svehla, Roger A.; and Brokaw, Richard S.: Heat Capacity and the Lewis Number of a Reacting Gas. AIAA J., vol. 4, no. 1, Jan. 1966, pp. 182-184.

24. Brokaw, Richard S.: The Lewis Number. Progress in International Research on Thermodynamic and Transport Properties. Joseph F. Masi and Donald H. Tsai, eds., Academic Press, Inc., 1962, pp. 271-278.

25. Svehla, Roger A.: Thermodynamic and Transport Properties for the Hydrogen-Oxygen System. NASA SP-3011, 1964.

26. Wobser, R.; und Müller, Fr.: Die innere Riebung von Gasen und Dämpfen und ihre Messung im Höppler-Viskosimeter. Kolloid-Beihefte, vol. 52, nos. 6-7, 1941, pp. 165-276.

27. Trautz, Max; und Bauman, P. B.: Die Reibung, Warmeleitung und Diffusion in Gasmischungen II. - Die Reibung von H_2-N_2-und H_2-CO-Gemischen. Ann., Physik, vol. 2, ser. 5, 1929, pp. 733-736.

E

28. Ivakin, B. A.; and Suetin, P. E.: An Investigation of the Temperature Dependence of the Diffusion Coefficients of Gases. Soviet Phys.-Tech. Phys., vol. 9, no. 6, Dec. 1964, pp. 866-872.

29. Zeleznik, Frank J.; and Svehla, Roger A.: Rotational Relaxation in Polar Gases. II. J. Chem. Phys., vol. 53, no. 2, July 15, 1970, pp. 632-646.

30. Nyeland, Carl: Rotational Relaxation of Homonuclear Diatomic Molecules. J. Chem. Phys., vol. 46, no. 1, Jan. 1, 1967, pp. 63-67.

31. Parker, J. G.: Rotational and Vibrational Relaxation in Diatomic Gases. Phys. Fluids, vol. 2, no. 4, July-Aug. 1959, pp. 449-462.

32. Sather, Norman F.; and Dahler, John S.: Molecular Friction in Dilute Gases. III. Rotational Relaxation in Polyatomic Fluids. J. Chem. Phys., vol. 37, no. 9, Nov. 1, 1962, pp. 1947-1951.

33. Svehla, Roger A.: Estimated Viscosities and Thermal Conductivities of Gases at High Temperatures. NASA TR R-132, 1962.

34. Monchick, L.; and Mason, E. A.: Transport Properties of Polar Gases. J. Chem. Phys., vol. 35, no. 5, Nov. 1961, pp. 1676-1697.

35. Yun, K. S.; and Mason, E. A.: Collision Integrals for the Transport Properties of Dissociating Air at High Temperatures. Phys. Fluids, vol. 5, no. 4, Apr. 1962, pp. 380-386.

36. Vanderslice, J. T.; Weissman, Stanley; Mason, E. A.; and Fallon, R. J.: High-Temperature Transport Properties of Dissociating Hydrogen. Phys. Fluids, vol. 5, no. 2, Feb. 1962, pp. 155-164.

37. Krupenie, Paul H.; Mason, Edward A.; and Vanderslice, Joseph T.: Interaction Energies and Transport Coefficients of Li + H and O + H Gas Mixtures at High Temperatures. J. Chem. Phys., vol. 39, no. 10, Nov. 1963, pp. 2399-2408.

38. Svehla, Roger A.; and Brokaw, Richard S.: Thermodynamic and Transport Properties for the $N_2O_4 \rightleftharpoons 2NO_2 \rightleftharpoons 2NO + O_2$ System. NASA TN D-3327, 1966.

39. Amdur, I.; and Mason, E. A.: Properties of Gases at Very High Temperatures. Phys. Fluids, vol. 1, no. 5, Sept.-Oct. 1958, pp. 370-383.

40. Lee, Jerry S.; and Bobbitt, Percy J.: Transport Properties at High Temperatures of CO_2-N_2-O_2-Ar Gas Mixtures for Planetary Entry Applications. NASA TN D-5476, 1969.

41. Schneider, Manfred; und Schäfer, Klaus: Gasdiffusionsmessungen zwischen 273 und 1300° K. Ber. Bunsengesellschaft f. Physik, Chem., vol. 73, no. 7, 1969, pp. 702-706.

42. Malinauskas, A. P.: Gaseous Diffusion: The Systems He-Kr, Ar-Kr, and Kr-Xe. J. Chem. Phys., vol. 45, no. 12, Dec. 15, 1966, pp. 4704-4709.

43. Malinauskas, A. P.: Gaseous Diffusion. The Systems He-Ar, Ar-Xe, and He-Xe. J. Chem. Phys., vol. 42, no. 1, Jan. 1, 1965, pp. 156-159.

44. Walker, R. E.; and Westenberg, A. A.: Molecular Diffusion Studies in Gases at High Temperature. II. Interpretation of Results on the He-N_2 and CO_2-N_2 Systems. J. Chem. Phys., vol. 29, no. 5, Nov. 1958, pp. 1147-1153.

45. Amdur, I.; Mason, E. A.; and Jordan, J. E.: Scattering of High Velocity Neutral Particles. X. He-N_2; A-N_2. The N_2-N_2 Interaction. J. Chem. Phys., vol. 27, no. 2, Aug. 1957, pp. 527-531.

46. Walker, R. E.; and Westenberg, A. A.: Molecular Diffusion Studies in Gases at High Temperature. IV. Results and Interpretation of the CO_2-O_2, CH_4-O_2, H_2-O_2, CO-O_2, and H_2O-O_2 Systems. J. Chem. Phys., vol. 32, no. 2, Feb. 1960, pp. 436-442.

47. Davies, R. H.; Mason, E. A.; and Munn, R. J.: High-Temperature Transport Properties of Alkali Metal Vapors. Phys. Fluids, vol. 8, no. 3, Mar. 1965, pp. 444-452.

48. Belyayev, Yu. N.; and Leonas, V. B.: Kinetic Properties of Air and Other Gases at High Temperatures. NASA TT F-11837, 1968.

49. Amdur, I.; and Smith, Allan L.: Scattering of High-Velocity Neutral Particles. XV. He-H_2 and He-D_2. J. Chem. Phys., vol. 48, no. 2, Jan. 15, 1968, pp. 565-568.

50. Dymond, J. H.; and Alder, B. J.: Pair Potential for Argon. J. Chem. Phys., vol. 51, no. 1, July 1, 1969, pp. 309-320.

51. Samuilov, E. V.; and Voskresenskaya, N. V.: Interaction Cross Sections for C + O Atoms. High Temp., vol. 3, no. 6, Nov.-Dec. 1965, pp. 794-800.

TABLE I. - FORMAT OF THERMODYNAMIC AND TRANSPORT DATA

(a) THERMO (thermodynamic) data

Card order	Content	Format	Card column
1	THERMO	3A4	1 to 6
2	Temperature ranges for two sets of coefficients: lowest T, common T, and highest T	3F10.3	1 to 30
3	Species name	3A4	1 to 12
	Date	2A3	19 to 24
	Atomic symbols and formula	4(A2, F3.0)	25 to 44
	Phase of species (S, L, or G for solid, liquid, or gas, respectively)	A1	45
	Temperature range	2F10.3	46 to 65
	Integer 1	I15	80
4	Coefficients a_i(i = 1 to 5) in equations (3) to (5) (for upper temperature interval)	5(E15.8)	1 to 75
	Integer 2	I5	80
5	Coefficients in equations (3) to (5) (a_6 and a_7 for upper temperature interval and a_1, a_2, and a_3 for lower)	5(E15.8)	1 to 75
	Integer 3	I5	80
6	Coefficients in equations (3) to (5) (a_4, a_5, a_6, and a_7 for lower temperature interval)	4(E15.8)	1 to 60
	Integer 4	I20	80
(a)	Repeat cards numbered 1 to 4 in card column 80 for each species		
Final card	END (indicates end of thermodynamic data)	3A4	1 to 3

[a]Gaseous species and condensed species with only one condensed phase can be in any order. However, the sets for two or more condensed phases of the same species must be adjacent. If there are more than two condensed phases of a species, their sets must be either in increasing or decreasing order according to their temperature intervals.

TABLE I. - Concluded. FORMAT OF THERMODYNAMIC AND TRANSPORT DATA

(b) TRANSPORT data

Card type	Content[a]	Format	Card column
1	Identification of interaction: chemical formula of species 1, chemical formula of species 2, number of temperatures in table (NTP), code to indicate type of data (1 for transport and 2 for relaxation), and number of rotational degrees of freedom	2(3A4, 6X), 2I5, F24.1	1 to 70
[b]2	Tables of data: either transport data (temperature, viscosity cross section, A^*, and B^*) or relaxation data (temperature, rotational collision number, vibrational collision number, and dimensionless vibrational heat capacity (C_{vib}/R))	4F10.4	1 to 40
3	End card to indicate end of transport data; LAST written in card columns 1 to 4	A4	1 to 4

[a]Identification of interaction is done by giving chemical formula of particular species involved, whether they are the same or different. They may be specified in either order, inasmuch as the program assumes interaction A-B to be same as B-A. The number of rotational degrees of freedom is meaningful only for data of a pure species (interaction of the type A-A). The temperature schedule is arbitrary, provided the number of temperatures is not more than the maximum of 20. In addition, the data should be ordered in either an increasing or decreasing function of temperature, in order that interpolation within the table be meaningful. As a matter of input convenience, the Hirschfelder-Eucken approximation is denoted by setting the collision number equal to 0.0. If the vibrational heat capacity is not specified ($C_{vib}/R = 0$), the program will calculate a value assuming that the electronic heat capacity is zero and that the rotational heat capacity is classical. For polar molecules A^* should be corrected for resonant exchange of internal energy. See the main-text section TRANSPORT PROPERTY EQUATIONS for an explanation.

[b]There are NTP cards of type 2. They are followed by a card of either type 1 or type 3.

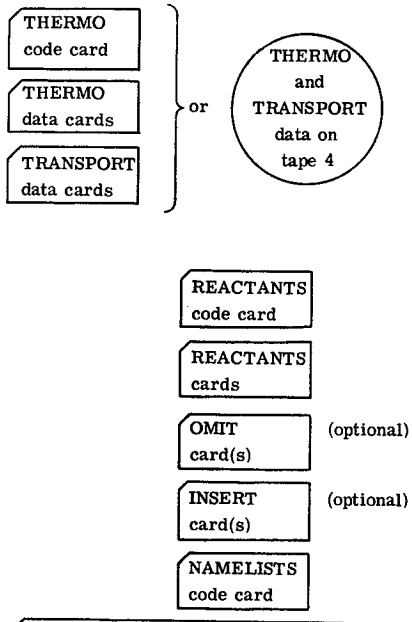

TABLE II. - PROGRAM INPUT

Problem	Namelist	Variables	
		Required	Optional
Assigned temperature and pressure (TP)	INPT2	TP = .TRUE. T(1 to 52); P(1 to 26)	NSQM, PSIA, or MMHG
Assigned enthalpy and pressure (HP)	INPT2	HP = .TRUE. P(1 to 26)	NSQM, PSIA, or MMHG
Assigned entropy and pressure (SP)	INPT2	SP = .TRUE. S0(1); P(1 to 26)	NSQM, PSIA, or MMHG
Assigned temperature and volume or density (TV)	INPT2	TV = .TRUE. T(1 to 52); V(1 to 26) or RHO(1 to 26)	
Assigned internal energy and volume or density (UV)	INPT2	UV = .TRUE. V(1 to 26) or RHO(1 to 26)	
Assigned entropy and volume or density (SV)	INPT2	SV = .TRUE. V(1 to 26) or RHO(1 to 26); S0(1)	
Detonation (DETN)	INPT2	DETN = .TRUE. P(1 to 26) (initial gas)	T(1 to 52)(initial gas); NSQM, PSIA, or MMHG
Shock (SHOCK)	INPT2	SHOCK = .TRUE. P(1 to 13) (initial T(1 to 13) gas)	NSQM, PSIA, or MMHG
	SHKINP	U1(1 to 13) or MACH1 (1 to 13)	INCDEQ = .FALSE. or INCDFZ = .FALSE.
Rocket (RKT)	INPT2	RKT = .TRUE. P(1 to 26) (chamber pressures)	T(1 to 52) (chamber); NSQM, PSIA, or MMHG
	RKTINP		EQL = .FALSE. or FROZ = .FALSE. NFZ PCP(1 to 22) SUPAR(1 to 13) SUBAR(1 to 13)

TABLE III. - REACTANTS CARDS

Card order	Content	Format	Card column
First	REACTANTS	3A4	1 to 9
Any	One card for each reactant species (maximum, 15). Each card contains		
	(1) Atomic symbols and formula numbers (maximum, five sets)[a]	5(A2,F7.5)	1 to 45
	(2) Relative weight[b] or number of moles	F7.5	46 to 52
	(3) Blank if (2) is relative weight, or M if (2) is number of moles	A1	53
	(4) Enthalpy or internal energy[a], cal/mole	F9.5	54 to 62
	(5) State: S, L, or G for solid, liquid, or gas, respectively	A1	63
	(6) Temperature associated with enthalpy in (4)	F8.5	64 to 71
	(7) F if fuel, or O if oxidant	A1	72
	(8) Density in g/cm^3 (optional)	F8.5	73 to 80
Last	Blank		

[a]Program will calculate the enthalpy or internal energy (4) for species in the THERMO data at the temperature (6) if zeros are punched in card columns 37 and 38.

[b]Relative weight of fuel in total fuels or oxidant in total oxidants. All reactants must be given either all in relative weights or all in number of moles. This number must never be zero.

TABLE IV. - LIST OF REACTANTS CARDS FOR SOME OXIDANTS AND FUELS

Chemical	Chemical formula (card columns 1 to 45)	Percent (cc 46-52)	Assigned enthalpy, cal/mole (cc 54-62)	(a)	Temperature, K (cc 64-71)	(b)	Density, g/cm^3 (cc 73-80)
Acetonitrile	C 2. H 3. N 1.	100.	12800.	L	298.15	F	.7857
Acetylene	C 2. H 2.	100.	49270.	L	192.60	F	.610
Air[c]	N 1.56176O .41959 AR.0009324O .000300	100.	-28.2	G	298.15	O	
Aluminum	AL1.	100.	0.	S	298.15	F	2.702
Ammonia(g)	N 1. H 3.	100.	-10970	G	298.15	F	
Ammonia(ℓ)	N 1. H 3.	100.	-17090	L	239.72	F	.676
Ammonium perchlorate	N 1. H 4. CL1. O 4.	100.	-70690	S	298.15	F	1.95
Aniline	C 6. H 7. N 1.	100.	7100.	L	298.15	F	1.02173
Argon	AR1.	100.	0.0	G	298.15	F	
Benzene	C 6. H 6.	100.	11718.	L	298.15	F	.8737
Beryllium	BE1.	100.	0.0	S	298.15	F	1.85
Butane	C 4. H 10.	100.	-36080.	L	272.65	F	.6012
1-butene	C 4. H 8.	100.	-5800	L	266.9	F	.6263
Chlorine(g)	CL2.	100.	0.	G	298.15	O	
Chlorine(ℓ)	CL2.	100.	-5391.	L	239.09	O	1.56
Chlorine trifluoride(g)	CL1. F 3.	100.	-39000.	G	298.15	O	
Chlorine trifluoride(ℓ)	CL1. F 3.	100.	-45680.	L	284.55	O	1.8517
Cyanogen(g)	C 2. N 2.	100.	73840.	G	298.15	F	
Cyanogen(ℓ)	C 2. N 2.	100.	67655.	L	252.01	F	.9537
Diborane	B 2. H 6.	100.	4970.	L	180.59	F	.4371
Ethane	C 2. H 6.	100.	-25008.	L	184.52	F	.5464
Ethyl alcohol	C 2. H 6. O 1.	100.	-66370.	L	298.15	F	.7893
Ethylene	C 2. H 4	100.	8100.	L	169.44	F	.5688
Ethylene oxide	C 2. H 4. O 1.	100.	-18840.	L	283.72	F	.8824
Ethylene polymer[d]	C 1. H 2.	100.	-6100.	S	298.15	F	.935
Fluorine(g)	F 2.	100.	0.	G	298.15	O	
Fluorine(ℓ)	F 2.	100.	-3098.	L	85.02	O	1.505
Graphite	C 1.	100.	0.	S	298.15	F	2.25
Helium	HE1.	100.	0.	G	298.15	F	
Heptane	C 7. H 16.	100.	-53630.	L	298.15	F	.67951
Hydrazine	N 2. H 4.	100.	12100.	L	298.15	F	1.0036

[a]Phase: S, solid; L, liquid; G, gas.

[b]Fuel, F; oxidant, O.

[c]Based on the following molar percents: N_2 = 78.0881, O_2 = 20.9495, Ar = 0.9324, CO_2 = 0.0300.

[d]Estimate based on paraffin hydrocarbon series.

TABLE IV. - Concluded. LIST OF REACTANTS CARDS FOR SOME OXIDANTS AND FUELS

Chemical	Chemical formula (card columns 1 to 45)	Percent (cc 46-52)	Assigned enthalpy, cal/mole (cc 54-62)	(a)	Temperature, K (cc 64-71)	(b)	Density, g/cm^3 (cc 73-80)
Hydrogen(g)	H 2.	100.	0.	G	298.15	F	
Hydrogen(ℓ)	H 2.	100.	-2154.	L	20.27	F	.0709
Hydrogen peroxide	H 2. O 2.	100.	-44880.	L	298.15	O	1.407
IRFNA[e]	H 1.57216N 1.62945O 4.69505F .02499	100.	-64860.	L	298.15	O	1.48
JP-5, ASTMA1[f]	C 1. H 1.9185	100.	-5300.	L	298.15	F	.807
JP-4, RP-1[g]	C 1. H 1.9423	100.	-5430.	L	298.15	F	.773
Lithium(ℓ)	LI1.	100.	1714.1	L	453.69	F	.512
Lithium(s)	LI1.	100.	0.	S	298.15	F	.534
Lithium perchlorate	LI1. CL1. O 4.	100.	-90880.	S	298.15	O	2.43
Methane(g)	C 1. H 4.	100.	-17895.	G	298.15	F	
Methane(ℓ)	C 1. H 4.	100.	-21390.	L	111.66	F	.4239
Methyl alcohol	C 1. H 4. O 1.	100.	-57040.	L	298.15	F	.78659
Monomethyl hydrazine	C 1. H 6. N 2.	100.	12900.	L	298.15	F	.874
Nitric acid	H 1. N 1. O 3.	100.	-41460.	L	298.15	O	1.5027
Nitrogen(g)	N 2.	100.	0.0	G	298.15	F	
Nitrogen(ℓ)	N 2.	100.	-2939.	L	77.35	F	.808
Nitrogen tetroxide	N 2. O 4.	100.	-4680.	L	298.15	O	1.431
Nitrogen trifluoride	N 1. F 3.	100.	-34100.	L	144.14	O	1.531
Nitromethane	C 1. H 3. N 1. O 2.	100.	-27030.	L	298.15	F	1.1371
Octane	C 8. H 18.	100.	-59740.	L	298.15	F	.69849
Oxygen(g)	O 2.	100.	0.0	G	298.15	O	
Oxygen(ℓ)	O 2.	100.	-3102.	L	90.18	O	1.149
Oxygen difluoride	O 1. F 2.	100.	1869.	L	127.88	O	1.521
Ozone(g)	O 3.	100.	34100.	G	298.15	O	
Ozone(ℓ)	O 3.	100.	30310.	L	162.64	O	1.449
Pentaborane	B 5. H 9.	100.	7740.	L	298.15	F	.6183
Perchloryl fluoride	CL1. O 3. F 1.	100.	-11350.	L	226.48	O	1.392
Propane	C 3. H 8.	100.	-30372.	L	231.08	F	.5808
n-propyl nitrate	C 3. H 7. N 1. O 3.	100.	-51270.	L	298.15	F	1.0538
Toluene	C 7. H 8.	100.	2867.	L	298.15	F	.86230
Unsymmetrical dimethylhydrazine	C 2. H 8. N 2.	100.	11900.	L	298.15	F	.783

[a]Phase: S, solid; L, liquid; G, gas.

[b]Fuel, F; oxidant, O.

[e]Inhibited red fuming nitric acid based on following weight percents: $HNO_3(\ell)$= 83.5, $N_2O_4(\ell)$= 14, $H_2O(\ell)$= 2, HF(g) = 0.5.

[f]Typical jet fuel having following properties: H/C weight ratio = 0.161, heat of combustion = 18 600 Btu/lb.

[g]Typical jet fuel having following properties: H/C weight ratio = 0.163, heat of combustion = 18 640 Btu/lb.

TABLE V. - VARIABLES IN INPT2 NAMELIST

Variable	Dimension	Type	Common label	Value before read	Definition and comments
KASE	1	I	INDX	0	Optional assigned number associated with case
P	26	R	POINTS	0	Assigned pressures: chamber pressures for rocket problems; values in atm unless PSIA, NSQM, or MMHG = T (see below)
NSQM	1	L	----------	FALSE	Values in P array in N/m^2 [b]
PSIA	1	L	----------	FALSE	Values in P array in psia units[b]
MMHG	1	L	----------	FALSE	Values in P array in mm Hg units[b]
V	26	R	POINTS	0	Volume, cm^3/g
RHO	26	R	POINTS[a](P)	0	Density, g/cm^3
T	26	R	POINTS	0	Assigned temperature, K
MIX	15	R	MISC[a](OXF)	0	Values of equivalence ratios if ERATIO = T; oxidant-to-fuel weight ratio if OF = T; percent fuel by weight if FPCT = T; and fuel-to-air weight ratio if FA = T
ERATIO	1	L	MISC	FALSE	Equivalence ratios given in MIX[b]
OF	1	L	MISC	FALSE	Oxidant-to-fuel weight ratios given in MIX[b]
FPCT	1	L	MISC	FALSE	Percent fuel by weight given in MIX[b]
FA	1	L	----------	FALSE	Fuel-to-air weight ratios given in MIX[b]
TRACE	1	R	MISC	0 (5. E-9 for SHOCK problem)	Option to print mole fractions ≥ TRACE in special E-format
IONS	1	L	INDX	FALSE	Consider ionic species[b]
IDEBUG	1	I	INDX	0	Print intermediate output for all points indexed ≥ integer value
TP	1	L	INDX	FALSE	Assigned temperature and pressure problem[b]
HP	1	L	INDX	FALSE	Assigned enthalpy and pressure problem[b]
SP	1	L	INDX	FALSE	Assigned entropy (S0) and pressure problem[b]
S0	1	R	MISC	0	Assigned entropy, cal/(g)(K)
TV	1	L	INDX	FALSE	Assigned temperature and volume (or density) problem[b]
UV	1	L	INDX	FALSE	Assigned internal energy and volume (or density) problem[b]
SV	1	L	INDX	FALSE	Assigned entropy (S0) and volume (or density) problem[b]
RKT	1	L	----------	FALSE	Rocket problem[b]
DETN	1	L	----------	FALSE	Detonation problem[b]
SHOCK	1	L	INDX	FALSE	Shock problem[b]
TRNSPT	1	L	CONTRL	TRUE	Transport properties included with the calculations[b]
PUNCH	1	L	CONTRL	FALSE	Punched cards of calculations included with output[b]
NODATA	1	L	CONTRL	FALSE	Message concerning missing transport data not printed[b]
FROZN	1	L	CONTRL	FALSE	Frozen transport properties calculated for the current point[b]

[a]Equivalenced to variable given in parentheses.

[b]If variable is set to be TRUE.

TABLE VI. - VARIABLES IN RKTINP NAMELIST[a]

Variable	Dimension	Type	Common label	Value before read	Definition and comments
EQL	1	L	PERF	TRUE	Calculate rocket performance assuming equilibrium composition during expansion[b]
FROZ	1	L	PERF	TRUE	Calculate rocket performance assuming frozen composition during expansion[b]
NFZ	1	I	PERF	1	Freezing point; must be ≤13
PCP	26	R	PERF	0	Ratio of chamber pressure to exit pressure; list should not include values for the chamber and throat; storage allows for 22 values
SUBAR	13	R	PERF	0	Subsonic area ratios
SUPAR	13	R	PERF	0	Supersonic area ratios

[a]Required for rocket problems only.
[b]Set variable to be FALSE if these calculations are not desired.

TABLE VII. - VARIABLES IN SHKINP NAMELIST[a]

Variable	Dimension	Type	Value before read	Definition and comments
INCDEQ	1	L	TRUE	Calculate incident shock parameters assuming equilibrium compositions[b]
INCDFZ	1	L	TRUE	Calculate incident shock parameters assuming frozen compositions[b]
REFLEQ	1	L	FALSE	Calculate reflected shock parameters assuming equilibrium composition[c]
REFLFZ	1	L	FALSE	Calculate reflected shock parameters assuming composition frozen at incident composition[c]
U1	13	R	0	Shock velocity in m/sec (not required if values of Mach1 are listed)
MACH1	13	R	0	Ratio of shock velocity to the velocity of sound in the unshocked gas (not required if values of U1 are listed)

[a]Required for shock problems only.
[b]Set variable to be FALSE if these calculations are not desired.
[c]If variable is set to be TRUE.

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TABLE VIII. - SOURCES OF TRANSPORT DATA

Interaction	Temperature range of data included with program, K	Method (a)	Interaction	Temperature range of data included with program, K	Method (a)	Interaction	Temperature range of data included with program, K	Method (a)
Ar-Ar	200 to 5000	21	CO_2-SF_6	200 to 5000	12	K-K	1000 to 10 000	18
Ar-CO	200 to 8000	9	CS_2-CS_2	↓	1	Kr-Kr	200 to 5000	10
Ar-CO_2	200 to 8000	11	C_2H_2-C_2H_2	↓	↓	Kr-Xe	200 to 5000	14
Ar-H_2	200 to 5000	12	C_2H_4-C_2H_4	↓	↓	Li-Li	1500 to 10 000	18
Ar-He	200 to 5000	15	C_2H_6-C_2H_6	↓	↓	N-N	1000 to 10 000	4
Ar-Kr	200 to 5000	14	C_2N_2-C_2N_2	↓	↓	N-NO	1000 to 8000	11
Ar-N	1000 to 8000	11	C_6H_6-C_6H_6	↓	↓	N-N_2	1000 to 10 000	4
Ar-NO	200 to 8000	↓	Cl_2-Cl_2	↓	↓	N-O	1000 to 10 000	4
Ar-N_2	200 to 8000	↓	Cs-Cs	1000 to 10 000	18	ND_3-ND_3	200 to 5000	2
Ar-O	1000 to 8000	↓	DCl-DCl	200 to 5000	3	NH_3-NH_3	↓	2
Ar-O_2	200 to 8000	↓	DF-DF	200 to 5000	2	NO-NO	↓	1
Ar-SF_6	200 to 5000	12	D_2O-D_2O	300 to 5000	2	NO-NO_2	↓	8
Ar-Xe	↓	15	F_2-F_2	200 to 5000	1	NO-O	1000 to 10 000	4
BCl_3-BCl_3	↓	1	H-H	1000 to 10 000	5	NO-N_2O_4	200 to 2000	8
BF_3-BF_3	↓	1	H-H_2	1000 to 10 000	5	NO_2-NO_2	200 to 5000	↓
Br_2-Br_2	↓	1	H-He	2000 to 10 000	19	NO_2-O_2	200 to 5000	↓
C-O	1000 to 10 000	22	H-Li	1000 to 10 000	6	NO_2-N_2O_4	200 to 2000	↓
CCl_4-CCl_4	200 to 5000	1	H-O	1000 to 10 000	6	N_2-N_2	200 to 10 000	4
CF_4-CF_4	↓	1	HBr-HBr	200 to 5000	2	N_2-O	1000 to 10 000	4
$CHCl_3$-$CHCl_3$	↓	3	HCN-HCN	↓	2	N_2-O_2	200 to 10 000	4
CH_3Cl-CH_3Cl	↓	3	HCl-HCl	↓	3	N_2-SF_6	200 to 5000	12
CH_3OH-CH_3OH	↓	3	HF-HF	↓	2	N_2O-N_2O	200 to 5000	1
CH_4-CH_4	↓	1	HI-HI	↓	1	N_2O_4-N_2O_4	200 to 2000	8
CH_4-O_2	↓	17	H_2-H_2	200 to 10 000	5	N_2O_4-O_2	200 to 2000	8
CO-CO	200 to 10 000	9	H_2-H_2O	300 to 5000	7	Na-Na	1000 to 10 000	18
CO-CO_2	200 to 8000	↓	H_2-He	2000 to 10 000	20	Ne-Ne	200 to 5000	10
CO-H_2	200 to 5000	↓	H_2-N_2	200 to 5000	13	O-O	1000 to 10 000	4
CO-He	200 to 5000	↓	H_2-OH	500 to 5000	7	O-O_2	1000 to 10 000	4

M M M

CO-N	1000 to 10 000		H_2-O_2	200 to 5000	7	OH-OH	500 to 5000	7
CO-N_2	200 to 10 000		H_2-SF_6	200 to 5000	12	OH-O_2	500 to 5000	7
CO-O	1000 to 10 000		H_2O-H_2O	300 to 5000	2	O_2-O_2	200 to 10 000	4
CO-O_2	200 to 10 000		H_2O-O_2	300 to 5000	7	Rb-Rb	1000 to 10 000	18
CO-SF_6	200 to 5000	12	H_2S-H_2S	200 to 5000	2	SF_6-SF_6	200 to 5000	1
COS-COS	200 to 5000	1	He-He		10	SO_2-SO_2		2
CO_2-CO_2	200 to 8000	11	He-Kr		14	SiF_4-SiF_4		1
CO_2-H_2	200 to 5000	13	He-N_2		16	SiH_4-SiH_4		1
CO_2-NO	200 to 8000	11	He-SF_6		12	UF_6-UF_6		1
CO_2-N_2	200 to 8000		He-Xe		15	Xe-Xe		10
CO_2-O	1000 to 8000		I_2-I_2		1			
CO_2-O_2	200 to 8000							

[a]Methods used to obtain transport data:

1. Lennard-Jones (12-6) potential. Parameters were taken from reference 33.
2. Stockmayer (12-6-3) potential. Parameters were obtained from reference 29. Equations for resonant correction were obtained from reference 20.
3. Same as previous method, except that parameters were obtained from reference 34.
4. Reference 35. Data were extended to lower temperatures in some cases by using the potential energy parameters of reference 35.
5. Reference 36. Data were extended to lower temperatures for H_2-H_2 by using the potential energy parameters of reference 36.
6. Reference 37.
7. Reference 25. Data were extended to lower temperatures in some cases by using the potential energy parameters of reference 25.
8. Lennard-Jones (12-6) potential. Parameters were obtained from reference 38.
9. Cross-section data for interactions of the type CO-X were assumed to be the same as those for interactions of the type N_2-X.
10. Data were obtained directly from the available transport property measurements. The cross sections were selected in order to adequately reproduce both the viscosity and thermal conductivity data. At higher temperatures the cross-section data were smoothed into the results obtained from molecular beam scattering measurements (ref. 39).
11. Reference 40. Data were extended to lower temperatures in some cases by using the potential energy parameters of reference 40.
12. Exponential-6 potential. Parameters were taken from reference 28.
13. Lennard-Jones (12-6) potential. Parameters were taken from reference 41.
14. Lennard-Jones (12-6) potential. Parameters were taken from reference 42.
15. Lennard-Jones (12-6) potential. Parameters were taken from reference 43.
16. Exponential-6 potential. Parameters were taken from reference 28. Experimental diffusion data (ref. 44) and molecular beam scattering measurements (ref. 45) were used.
17. Exponential-6 potential. Parameters were taken from reference 46.
18. Reference 47.
19. Reference 48.
20. Reference 49.
21. Reference 50. Method 10 was used at higher temperatures.
22. Reference 51.

TABLE IX. - ROTATIONAL COLLISION NUMBERS

Molecule	Z_{rot}[a]	Source[b]
Ar	----------	Atom with no rotational energy modes
BCl_3	1	Obtained by fitting thermal conductivity data
BF_3	1	↓
Br_2	2	
CCl_4	1	
CF_4	1	
$CHCl_3$	908 to 26 581	Reference 29[b]
CH_3Cl	20 to 406	Reference 29[b]
CH_3OH	19 to 401	Reference 29[b]
CH_4	8	Obtained by fitting thermal conductivity data
CO	2	↓
COS	HE	
CO_2	3	
CS_2	HE	
C_2H_2	1	
C_2H_4	3	
C_2H_6	HE	
C_2N_2	2	Equation (44) using $Z_{rot}(N_2)$ as a reference
C_6H_6	HE	Obtained by fitting thermal conductivity data
Cs	----------	Atom with no rotational energy modes
Cl_2	1	Obtained by fitting thermal conductivity data
DCl	46 to 1084	Reference 29[b]
DF	4.3 to 22	Reference 29[b]
D_2O	13 to 37	Reference 29[b]
F_2	3	Obtained by fitting thermal conductivity data
H	----------	Atom with no rotational energy modes
HBr	485 to 6099	Reference 29[b]
HCN	2.8 to 10.5	↓
HCl	61 to 1349	
HF	5.7 to 27	
HI	HE	Equation (44) using $Z_{rot}(I_2)$ as a reference

[a]HE refers to Hirschfelder-Eucken approximation.

[b]Calculations of theoretical collision numbers were extended to cover the temperature range shown in table VIII.

TABLE IX. - Concluded. ROTATIONAL COLLISION NUMBERS

Molecule	Z_{rot} [a]	Source [b]
H_2	12	Obtained by fitting thermal conductivity data
H_2O	15 to 40	Reference 29[b]
H_2S	168 to 3393	Reference 29[b]
He	----------	Atom with no rotational energy modes
I_2	1	Obtained by fitting thermal conductivity data
K	----------	Atom with no rotational energy modes
Kr	----------	↓
Li	----------	↓
N	----------	↓
ND_3	12 to 193	Reference 29[b]
NH_3	16 to 235	Reference 29[b]
NO	2	Obtained by fitting thermal conductivity data
NO_2	3	↓
N_2	8	↓
N_2O	3	↓
N_2O_4	1	Equation (44) using $Z_{rot}(NO_2)$ as a reference
Na	--------	Atom with no rotational energy modes
Ne	--------	Atom with no rotational energy modes
O	--------	Atom with no rotational energy modes
OH	8	Estimated
O_2	8	Obtained by fitting thermal conductivity data
Rb	--------	Atom with no rotational energy modes
SF_6	1	Obtained by fitting thermal conductivity data
SO_2	28 to 657	Reference 29[b]
SiF_4	1	Obtained by fitting thermal conductivity data
SiH_4	9	Equation (44) using $Z_{rot}(CH_4)$ as a reference
UF_6	2	Equation (44) using $Z_{rot}(SF_6)$ as a reference
Xe	--------	Atom with no rotational energy modes

[a]HE refers to Hirschfelder-Eucken approximation.

[b]Calculations of theoretical collision numbers were extended to cover the temperature range shown in table VIII.

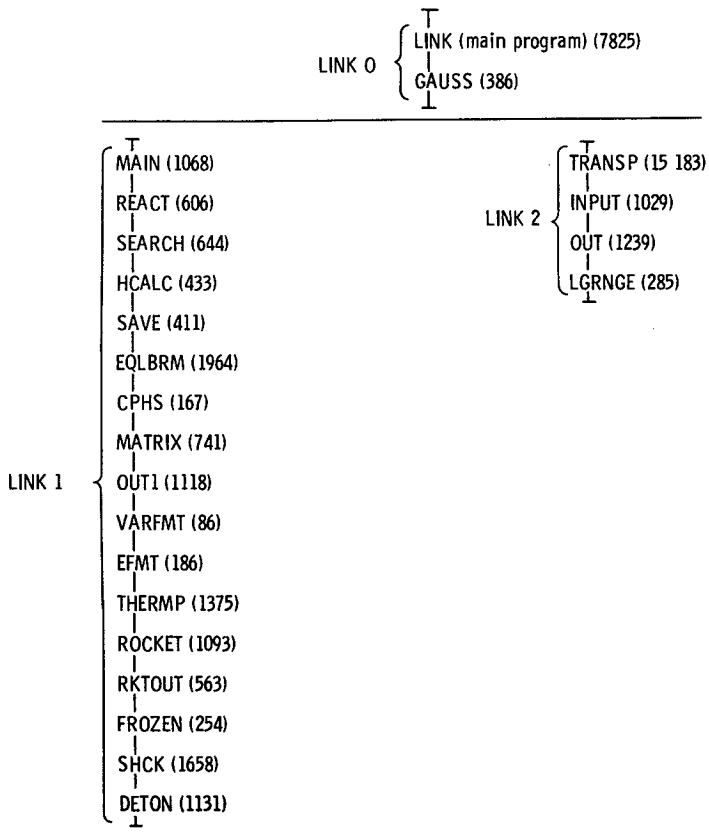

Figure 1. - Overlay structure of TRAN72 computer program for IBM 7094.

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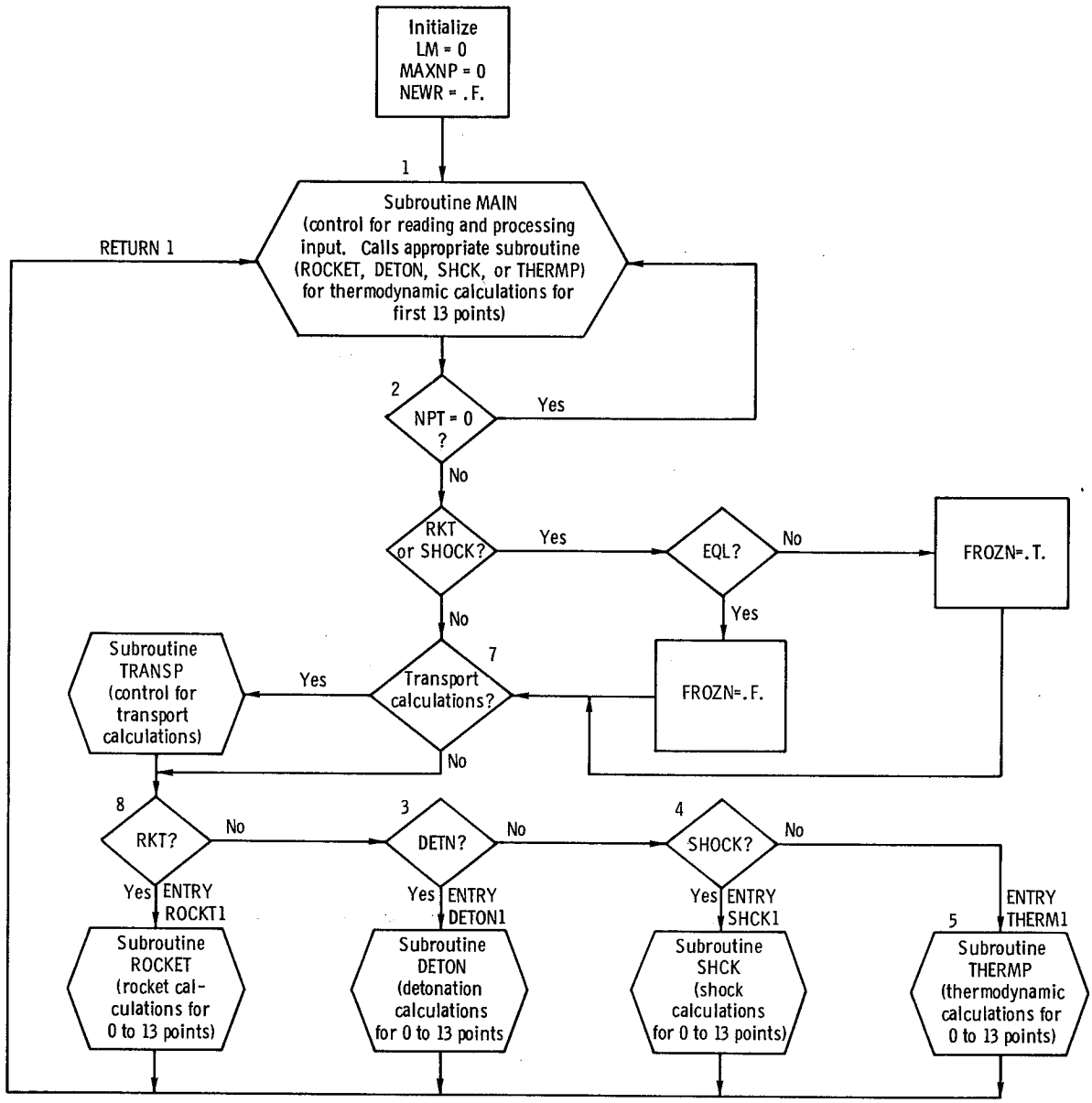


Figure 2. - Main program LINK.

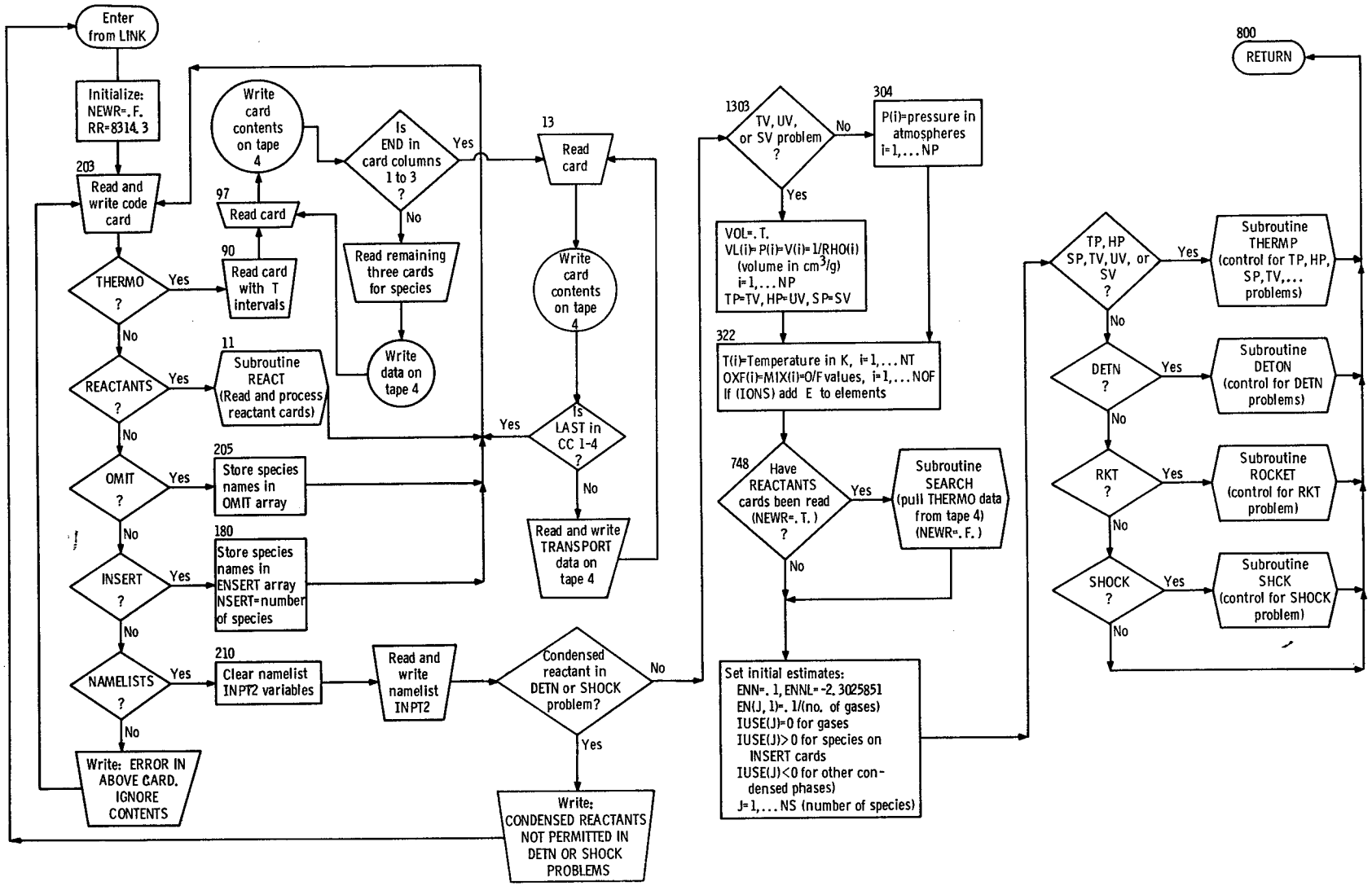


Figure 3. - Subroutine MAIN.

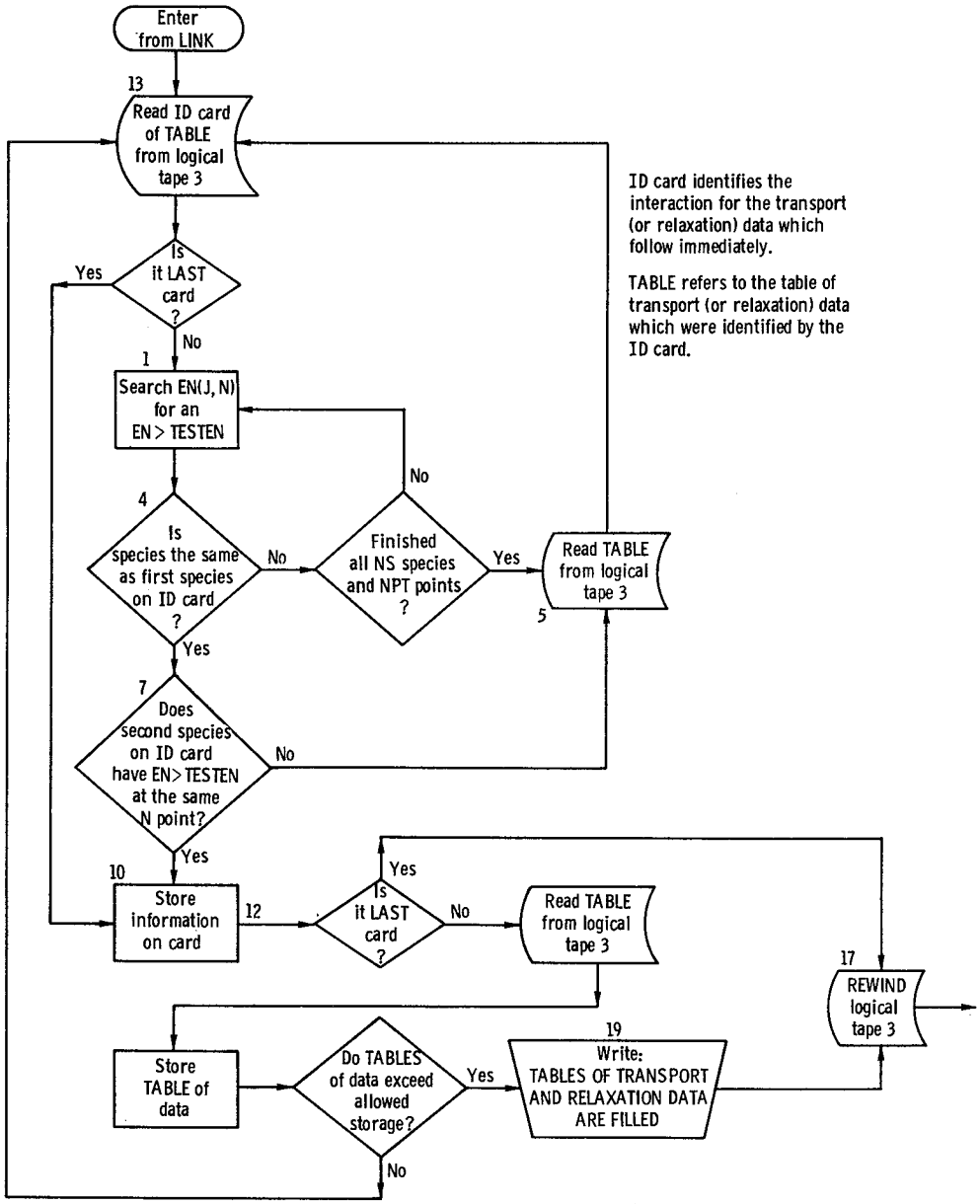
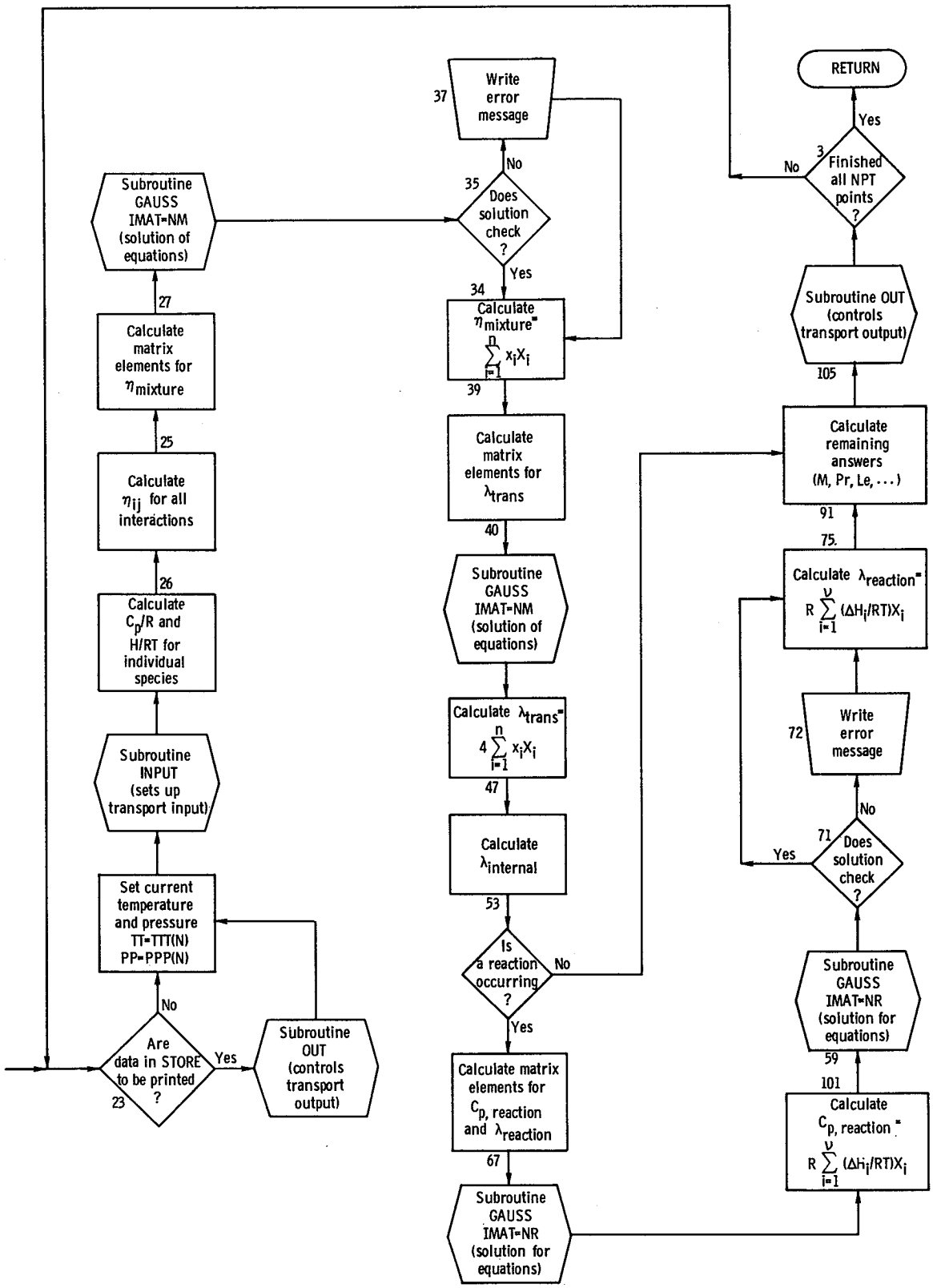

Enter from LINK
13
Read ID card of TABLE from logical tape 3
Is it LAST card ?
Yes
No
1
Search EN(J, N) for an EN > TESTEN
4
Is species the same as first species on ID card ?
No
Finished all NS species and NPT points ?
No
Yes
Read TABLE from logical tape 3
5
Yes
7
Does second species on ID card have EN > TESTEN at the same N point?
No
Yes
10
Store information on card
12
Is it LAST card ?
Yes
No
Read TABLE from logical tape 3
17
REWIND logical tape 3
Store TABLE of data
Do TABLES of data exceed allowed storage?
Yes
19
Write: TABLES OF TRANSPORT AND RELAXATION DATA ARE FILLED
No
ID card identifies the interaction for the transport (or relaxation) data which follow immediately.
TABLE refers to the table of transport (or relaxation) data which were identified by the ID card.

Figure 4. -



Subroutine TRANSP.

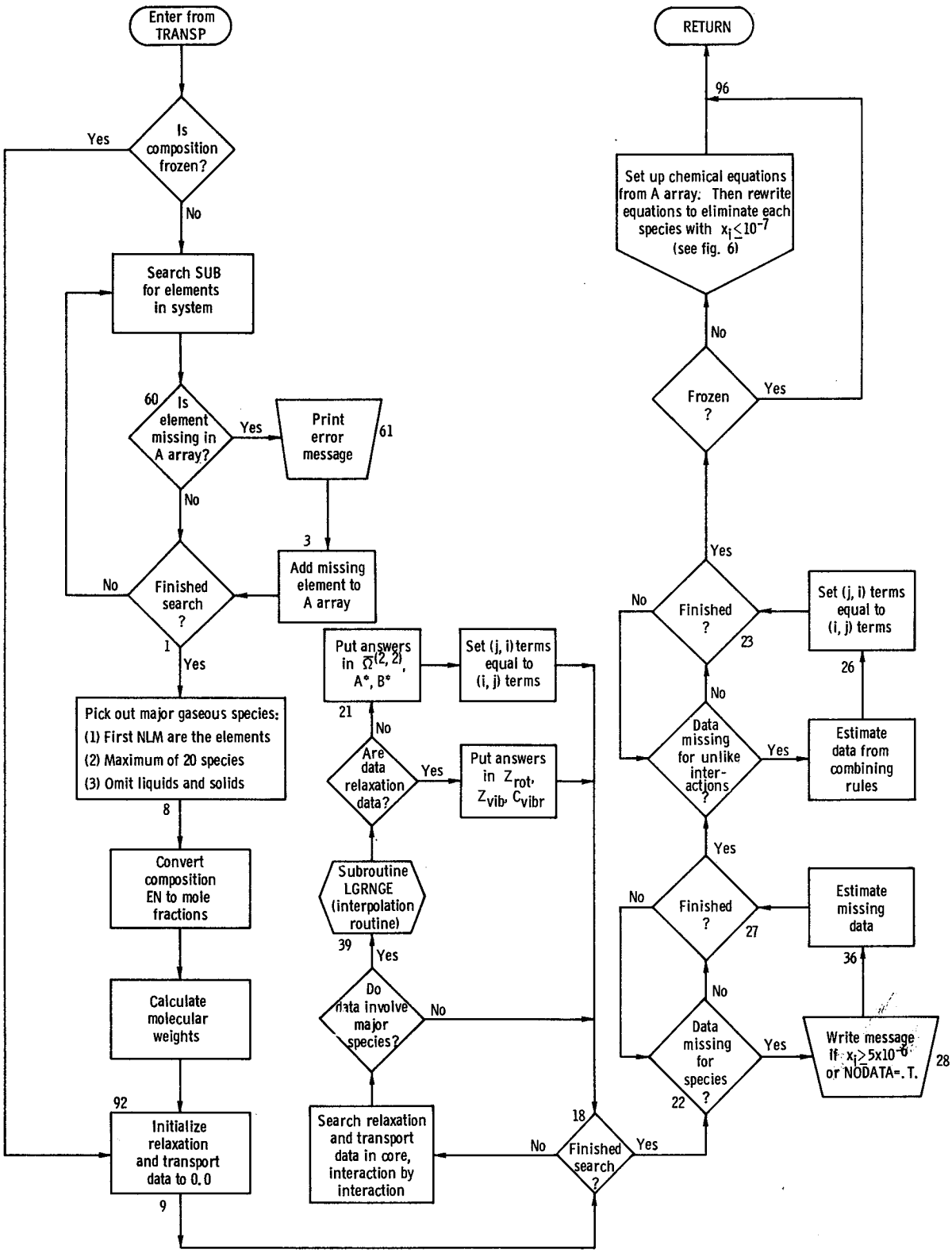


Figure 5. - Subroutine INPUT.

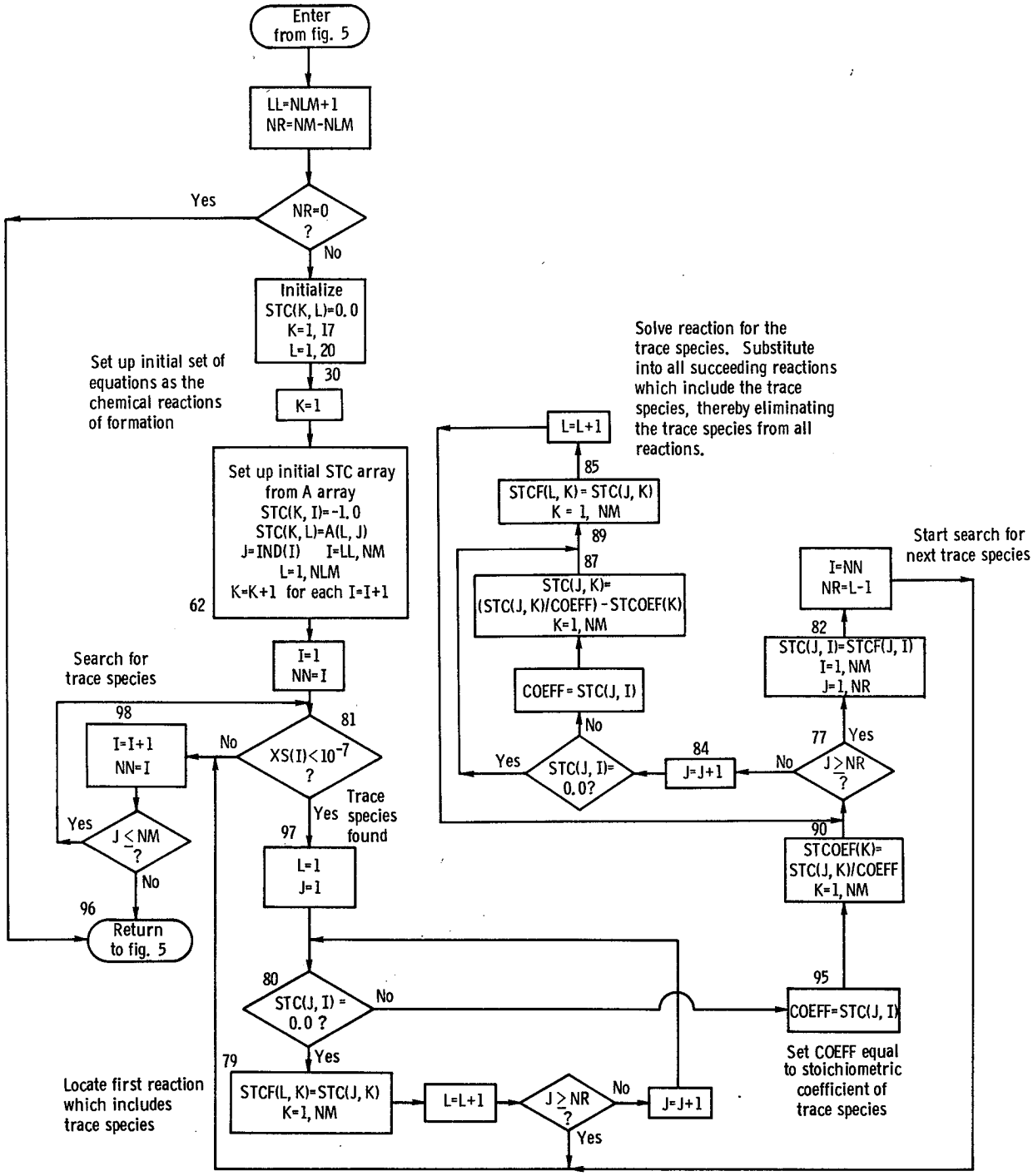


Figure 6. - Rewrite equations to eliminate trace species section in subroutine INPUT.

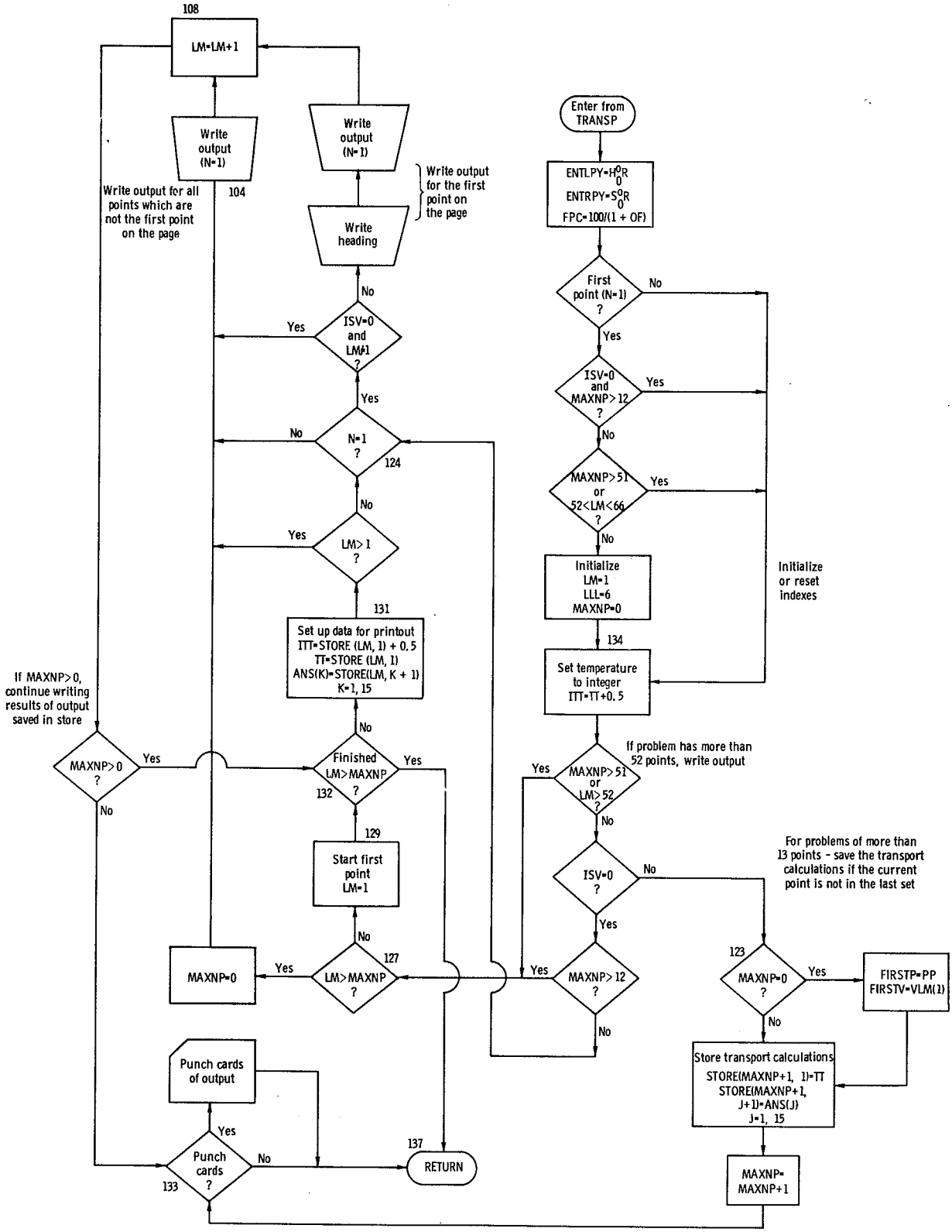


Figure 7. - Subroutine OUT.