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THEORETICAL GUN PROPELLANT THERMOCHEMICAL EVALUATION

GUNS AND ROCKETS BRANCH
ADVANCED DEVELOPMENT DIVISION

TECHNICAL REPORT AFATL-TR-71-11

JANUARY 1971

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13 ABSTRACT

A computer program is presented for the computation of chemical equilibrium reaction products associated with gun propellant combustion. The program as developed at the Air Force Armament Laboratory was based on a code used by the NASA Lewis Research Center. The program provides a first approximation of flame temperature, specific heat ratio, impetus, and mean molecular weight of the combustion products. A simplified users manual is presented for thermochemical programs and for the program to generate specific heat polynomials from JANAF tabular data.

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Theoretical Gun Propellant Thermochemical Evaluation

Otto K. Heiney

FOREWORD

This report has been generated under the advanced gun propellant evaluation analysis portion of Project 62602F 2560 and is presented as a state of the art advancement that can be applied to gun propellant research efforts. The study was conducted during the period February 1970 to January 1971.

This technical report has been reviewed and is approved.

Charles Petrides
CHARLES PETRIDES
Chief, Advanced Development Division

ABSTRACT

A computer program is presented for computing the chemical equilibrium reaction products associated with gun propellant combustion. This program will provide a good first approximation of flame temperature, specific heat ratio, impetus, and mean molecular weight of the combustion products. The program as developed at the Air Force Armament Laboratory was based on a code used by the National Aeronautics and Space Administration Lewis Research Center. The minor changes to the program are discussed, some results from advanced solid propellant formulations calculations are presented, and a form of users manual for thermochemical programs and for the program to generate specific heat polynomials from JANAF tabular data is presented.

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LIST OF ABBREVIATIONS AND SYMBOLS

C_p	Specific heat at constant pressure
C_v	Specific heat at constant volume
E	Internal energy
F_p	Propellant impetus
G	Gibbs free energy
H	Enthalpy
K	Gas conductivity
M	Molecular weight
P	Pressure
R	Gas constant
S	Entropy
T	Temperature
T_{FP}	Flame temperature at constant pressure
T_{FV}	Flame temperature at constant volume
V	Volume
X_i	Mole fraction
γ	Specific heat ratio
σ	Leonard-Jones force constant
Ω	Leonard-Jones force constant
μ	Gas viscosity

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SECTION I

INTRODUCTION

The field of gun propellant development, which had been relatively static for many years, has recently begun to attract increased attention. The availability of an accurate theoretical thermochemical propellant performance computer program is of central importance to informed research and development efforts in this field. As a formulation screening tool, a few dollars of machine time can save hundreds of dollars of laboratory small-batch-mix effort by eliminating unpromising candidate formulations and providing a good first approximation to the primary important propellant parameters. These would include flame temperature, specific heat ratio, impetus, and mean molecular weight of the combustion products. To most expediently obtain a computer program for computing the chemical equilibrium reaction products, the Air Force Armament Laboratory modified an existing free-energy minimization rocket propellant performance program. The program selected was the one used by the National Aeronautics and Space Administration Lewis Research Center. This code[1] has a background of almost ten years of successful application. In addition, it was readily available and the JANAF specific heat data could be easily applied to the thermodynamic data tape. The program, as modified for gun propellant applications, was checked against established experimental data and other analytic chemical equilibrium computing techniques, with excellent agreement. Additionally, an algorithm was added which computes combustion gas viscosity and thermal conductivity by a Leonard-Jones potential technique.

The following sections of this report discuss the minor changes made to the Lewis approach, give some results from advanced solid propellant formulation calculations, and provide a form of users manual for the thermochemical programs and for the program to generate specific heat polynomials form JANAF tabular data[2]. Appendix I presents the Lewis program listing and Appendix II presents the polynomial fit program used at the Armament Laboratory.

SECTION II

FREE ENTHALPY EQUATIONS

This report will not discuss the mathematical techniques of chemical equilibrium computations. This task has effectively been accomplished in a recently issued monograph[3] which discusses in detail not only the Lewis technique but also several other commonly used approaches. This report will demonstrate only that, at chemical equilibrium, the Gibbs free energy, G, (or free enthalpy) will be a minimum.

From the First Law of Thermodynamics, in an irreversible process:

$$dE + pdv - Tds<0 \tag{1}$$

or at equilibrium

$$dE + pdv - Tds=0 \tag{2}$$

For a constant pressure and temperature, equation (2) becomes

$$d(E + pv - Ts) =0 \tag{3}$$

$$G_T = H_T - T_1S_1 \tag{4}$$

Equation (4) establishes the relation that the Gibbs free energy will be a minimum at equilibrium, and when coupled with the atomic species mass conservation equations, it provides a sufficient set for solution of the combu tion species concentration and flame temperature (if the combustion pressure is specified). Then, to set up a minimization algorthm only requires a value for the heat of formation of the reactant compounds and tabular or polynomial data for the specified heat, C_p, enthalpy, H_T, and entropy, S_T, of the possible combustion products. These thermodynamic data can be obtained from reference 2 for most combustion products of interest: as

$$H_T - H_{298} = \int_{298}^{T} C_p \, dT \tag{5}$$

$$\text{and} \quad S_T - S_{298} = \int_{298}^{T} \frac{C_p}{T} \, dT \tag{6}$$

Selecting a polynomial form for C_p, the terms H_T and S_T can be conveniently fitted to similar polynomials by performing the indicated integrations

$$\frac{C_p}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4 \tag{7}$$

$$\frac{H_T}{RT} = a_1 + 1/2\ a_2T + 1/3\ a_3T^2 + 1/4\ a_4T^3 + 1/5\ a_5T^4 + a_6/T \tag{8}$$

$$\frac{S_T}{R} = a_1 LnT + a_2T + 1/2\ a_3T^2 + 1/3\ a_4T^3 + 1/4\ a_5T^4 + a_7 \tag{9}$$

For a more precise fit, the Lewis program utilizes two sets of coefficients for each species, one in the temperature range 0° to 1000°K and the other from 1000° to 6000°K. Limits of species existence can be placed on the propellant data to restrict the range of polynomial applicability.

The primary change made to the Lewis algorithm was to additionally develop an approximate isochoric temperature from the isobaric temperature provided by the program. This requires the assumption that approximately the same species would form either in an isochoric or isobaric process, providing a similar total heat release. If these assumptions are warranted, then:

$$Q_R = C_pT_{Fp} \tag{10}$$

$$Q_R = C_VT_{FV} \tag{11}$$

$$T_{FV} = C_p/C_VT_{Fp} = \gamma T_{Fp} \tag{12}$$

Once the isochoric flame temperature and mean molecular weight of the combustion products are known, the impetus is simply

$$F_p = \frac{R}{M}\ T_{FV} \tag{13}$$

where R = 2780 ft-lbs/lb-mole-°K

The program also computes the constitutive products mole fractions as a function of the pressure ratio (or, for a gun system, of the velocity) if quasi-isentropic conditions are assumed.

Equation (13) indicates the importance of developing advanced propellants with lower molecular weight combustion products, if the impetus of a propellant is to be increased without a corresponding flame temperature increase. High propellant flame temperatur s are, of course, the prime limiting factor in developing an acceptable barrel life for automatic aircraft cannon having a high performance and a high rate of fire. Current single-base solid gun propellants display molecular weights in the order of 25. Table I illustrates the distinctive flame temperature advantage of lower molecular weights in obtaining cooler combustion conditions without sacrificing energy output.

TABLE I. FLAME TEMPERATURES AS A FUNCTION OF MOLECULAR WEIGHT AND IMPETUS

Molecular Weight, Atomic Mass Units	Flame Temperature, °K, at Impetus, Ft-lb/lb			
	325,000	350,000	375,000	400,000
25	2980	2150	3380	3500
22	2570	2770	2970	3170
20	2340	2620	2700	2880
19	2220	2390	2570	2740
18	2110	2270	2430	2590
17	1990	2140	2290	2450

The very favorable performance data indicated by the lower right-hand entries in Table I are responsible for the continued advanced solid gun propellant development efforts. The test cases described in the following sections have resulted from calculations of two of the formulations now under contract investigation and from a comparison of results of two theoretical computations with experimental measurements of inservice propellants. All computations are performed at a standard reference pressure of 5,000 psia.

The first requirement for free energy computations is a reliable list of heats of formations for the constituents to be considered. Table II provides this data for the ingredients in the formulations discussed in this report. Additional tables are available in references 4 and 5.

TABLE II. HEATS OF FORMATION

CONSTITUENT	EMPIRICAL FORMULA	HEATS OF FORMATION KILOCALORIES PER MOLE
Ammonium Nitrate	$H_4 O_3 N_2$	-88.1
CTPB	$C_7 H_{11} O_{0.2} N_{0.02}$	-5.0
Dibutylphthalate	$C_{18} H_{14} O_4$	-200.0
Diphenylamine	$C_{12} H_{11} N_1$	+27.6
DMDTH	$C_6 H_{14} O_6 N_4$	-94.0
Ethyl Acrylate	$C_5 H_8 O_2$	-87.3
Ethyl Alcohol	$C_2 H_6 O_1$	-66.3
Ethyl Centralite	$C_{17} H_{20} O_1 N_2$	-34.2
Ethylene Dihydrazine	$C_2H_{10}N_4$	+31.2
Glycol Dinitrate	$C_2 H_4 O_6 N_2$	-58.7
Guanidine Nitrate	$C_1 H_6 O_3 N_4$	-79.3
HMX	$C_4 H_8 O_8 N_{812}$	+17.9
Nitrocellulose (12.6 percent N)	$C_{24} H_{30.2} O_{39.4} N_{9.8}$	-655.5
Nitrocellulose (12.7 percent N)	$C_{24} H_{30} O_{40} N_{10.0}$	-659.3
Nitrocellulose (13.15 percent N)	$C_{24} H_{29.5} O_{41.3} N_{10.6}$	-643.1
Nitrocellulose (13.75 percent N)	$C_{24} H_{29.3} O_{41.4} N_{10.7}$	-639.9
Nitroglycerine	$C_3 H_5 O_9 N_3$	-85.3
Nitroguanidine	$C_1 H_4 O_2 N_4$	-12.6
Polymethyl Vinyl Tetrazole	$C_4 H_6 N_4$	+52.4
RDX	$C_3 H_6 O_6 N_6$	+14.9
Potassium Sulfate	$K_2 S_1 C_4$	-338.5
Triacetin	$C_9 H_{14} O_6$	-307.0
Triazoethanol	$C_2 H_5 O_1 N_3$	+22.5
Triaminoguanidine Nitrate	$C_1 H_9 O_3 N_7$	-11.5
Water	$H_2 O_1$	-68.4

SECTION III

COMPUTATION OF VISCOSITY AND CONDUCTIVITY

For gun propellant applications, it is often quite important to determine a theoretical value for the combustion gas conductivity and viscosity. These are particularly necessary if the convective gun barrel heating characteristics of the propellants are to be evaluated. To accomplish this task, the Leonard-Jones potential technique[6] was applied.

The viscosity for a single constitutive species is given by:

$$\mu_1 = 2.6693 \times 10^{-5} \sqrt{MT} / \sigma^2 \Omega \tag{14}$$

where T is the temperature, M is the molecular weight, and σ and Ω are the Leonard-Jones force constants. The viscosity of the mixture is defined by

$$\mu_{MIX} = \sum_{i=1}^{n} \left(x_i \mu_i \right) \Big/ \left(\sum_{j=1}^{n} x_j \Phi_{ij} \right) \tag{15}$$

with n being the number of species considered and x_i being the mole fraction of the species. The value, Φ_{ij} is defined as

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left(1 + \frac{M_i}{M_j} \right)^{-1/2} \left[1 + \left(\frac{\mu_i}{\mu_j} \right)^{1/2} \left(\frac{M_j}{M_i} \right)^{1/4} \right]^2 \tag{16}$$

The thermal conductivity of a species is given as:

$$K_i = 1.9891 \times 10^{-4} \frac{\sqrt{T/M}}{\sigma^2 \Omega} \tag{17}$$

The mixture value is given as

$$K_{MIX} = \sum_{i=1}^{n} \left(x_i \ k_i \right) \Big/ \left(\sum_{j=1}^{n} x_j \ \Phi_{ij} \right) \tag{18}$$

This approach is strictly valid for only dilute mixtures of non-polar molecules. Five species are considered, (one of which, H_2O, is polar), and all have a dense gas system. Thus, the results contain only order of magnitude validity, but are none the less of value, considering the state of the art in mathematical modeling of the transient heat convection process in gun bores. Table III gives the species considered which are typically 98 to 99 percent of the combustion gas constitutients.

TABLE III. LEONARD-JONES POTENTIAL PARAMETERS (FORCE CONSTANTS)			
Species	Molecular Weight, Atomic Mass Units	Viscosity, Grams/cm-sec	Conductivity, Cal/cm-sec-K
H_2	2.016	2.915	38.0
N_2	28.02	3.749	79.8
CO	28.01	3.706	88.
CO_2	44.01	3.897	213.
H_2O	18.0	2.824	230.9

Table IV consists of the Ω-$\frac{KT}{\epsilon}$ relations needed for the solution of Equations (14) and (17). The first column contains values for the relatively non-polar species such as H_2, N_2, CO, and CO_2, while the second column has a corrected value for the highly polar H_2O.

TABLE IV. REDUCED CROSS SECTION						
KT/ ε	NON-POLAR	POLAR		KT/ε	NON-POLAR	POLAR
1.0	1.5938	2.6199		7	0.8725	0.8946
1.2	1.4568	2.4257		8	0.8536	0.8422
1.4	1.3557	2.2713		9	0.8378	0.8043
1.6	1.2800	2.1413		10	0.8242	0.7760
1.8	1.2216	2.0263		11	0.8123	0.7544
2.0	1.1751	1.9217		12	0.8017	0.7376
2.2	1.1377	1.8258		13	0.7922	0.7243
2.4	1.1066	1.7373		14	0.7836	0.7134
2.6	1.0803	1.6559		15	0.7756	0.7045
2.8	1.0579	1.5812		16	0.7883	0.6971
3.0	1.0385	1.5126		32	0.6939	0.6462
3.2	1.0214	1.4499		64	0.6262	0.6033
3.4	1.0063	1.3926		128	0.5634	0.5528
3.6	0.9928	1.3401		256	0.5056	0.5006
3.8	0.9807	1.2922		512	0.4528	0.4505
4.0	0.9696	1.2485				
5.0	0.9265	1.0797				
6 0	0.8960	0.9694				

SECTION IV

INPUT FOR GUN PROPELLANT PROGRAM

The input data for the gun propellant program (Appendix I) can be divided into four general groups having code names as follows:

1) Thermodynamic data for the reaction products (THERMØ data).
2) Data pertaining to the reactants or propellants (REACTANTS data).
3) Special options related to chemical species present in the combusted gas (ØMIT/INSERT data).
4) Namelist data including the type of problem, pressure ratio and area ratio schedules, various options, etc. (NAMELISTS data).

The required order of the data cards is:

1) One card with the code word THERMØ punched in columns 1 to 6.
2) THERMØ data.
3) REACTANTS card. Number of reactants right adjusted in columns 1 to 3 and number of cases right adjusted in columns 4 to 6.
4) ØMIT and/or INSERT data.
5) One card containing up to 80 columns of alphanumeric identification data.
6) NAMELISTS data.

For any particular problem there may be multiple REACTANTS cards. Each set of REACTANTS cards may be followed by multiple NAMELISTS input cards. Each type of input data is discussed in detail in the following sections.

1. THERMØ DATA

The thermodynamic data for the reaction products may be read either from cards or from magnetic tape. When tape input is used, both the THERMØ code card and all THERMØ data cards must be omitted. It is anticipated that most users will prefer the magnetic tape since this reduces the number of cards which must be handled. The card format for the THERMØ data is described in Section V. Use of the tape input requires no action on the part of the user, once the required data is established on the tape.

2. REACTANTS DATA

REACTANTS data is required for all problems. Following the code card there should follow one card for each reactant species being considered, with a maximum of 15 allowed. Each reactant card, after the code card, contains the following information:

a. The chemical formula for the species.

b. Either the number of moles of the reactant or the relative weight. The relative weight is the weight of each fuel or oxidizer expressed as a fraction of the total fuel or oxidizer.

c. The enthalpy of the species expressed in calories per mole. (This is not required for an assigned temperature problem. See Section IV.4 for description of assigned temperature problem.)

d. The state of the reactant (gas, liquid, or solid).

e. The temperature associated with the enthalpy.

f. Designation of each reactant species as either a fuel or an oxidizer. (The program then combines all fuels into an effective fuel and all oxidizers into an effective oxidizer.)

g. The reactant species density. (This information is optional and may be omitted. If densities are input for all reactants, the program calculates a density for the overall system.)

h. Multiple cases with identical reactants are identified by the reactants code card and the preceding data need not be repeated.

The reactant information is arranged on a card. Standard chemical alphabetic symbols are required for the chemical elements (i.e., H for hydrogen, HE for helium, LI for lithium, BE for beryllium, etc.). Each reactant may be composed of no more than five distinct chemical elements. Each chemical element is allowed two columns (columns 1 and 2, 10 and 11, 19 and 20, 28 and 29, and 37 and 38) for its symbol. For those elements whose symbol consists of a single letter, the symbol must be placed in the left-most (left adjusted) of the two columns. The formula number (the number of atoms of each element in a reactant) is to appear in the columns immediately following the chemical symbol (i.e., columns 3 to 9, 12 to 18, 21 to 27, 30 to 36, and 39 to 45). The formula number may appear anywhere within the seven column field, and a decimal point must be used for each number. Note that the exponent numeric form, or E format, may not be used here. Also note that for a given reactant an individual element may appear only once (empirical formula). Thus, a compound such as furfuryl alcohol, whose formula might be written as C4H3O·CH2OH to represent its structure, must be treated as though it were C5H6O2 or O2H6C5, etc. The order of the elements is immaterial for this program.

The relative weight of each reactant should be placed in columns 46 to 52. The number may appear anywhere in these columns, a decimal point must be used, and the exponent numeric form may not be used. If the number of moles of each species is input in these columns the same restrictions apply, but an additional bit of information, an M in column 53, must appear on the card. Column 53 is left blank for relative weights. Note that the relative weight and molar designations may not be mixed for any single problem.

The reactant enthalpy is placed in columns 54 to 62, and the units must be calories per mole. The number may appear anywhere in these columns, a decimal point must be used, and the exponent numeric form may not be used. A sign is required only if the enthalpy is negative. Obviously, this enthalpy must be consistent with the enthalpy base used for the THERMØ data. For the JANAF data, the enthalpy base is as follows: For each element, the phase, condensed or liquid, which is most stable at one atmosphere pressure is designated as a reference, or base, state. The heat of formation of this state at 298.15°K is arbitrarily specified as zero. Then all thermodynamic properties for other phases of the element, as well as for any compound containing the element, are referenced to the base state.

The initial state for each reactant is indicated by an S for solid, an L for liquid, or a G for gas in column 63. The initial reactant temperature, in degrees Kelvin, goes in columns 64 to 71. Both the initial state and temperature are used only to label the output printout and if they are omitted or input incorrectly, the calculations are not affected.

For all problem types (see Section IV.4) except a detonation problem, columns 73 to 70 are reserved for the reactant density in grams per cubic centimeter. The inputting of this data is optional, but if it is given, a decimal point must be used. For a detonation problem, columns 73 to 80 are used for the reactant specific heat at constant pressures. This data is required for each reactant for a detonation problem

3. ØMIT/INSERT DATA

The purpose of the ØMIT/INSERT option is as follows. The program considers as possible products all species in the THERMØ data which are consistent with the chemical system which was input on the REACTANTS cards. Occasionally, it may be desired to eliminate one or more species from consideration as possible products. This may be accomplished by placing the species chemical formula on an ØMIT card. Both gaseous and condensed species may be omitted.

Only the names of condensed species may appear on an INSERT card. The INSERT option has been included for two reasons. The less important of the two is that if it is known beforehand that one or more particular condensed species will be among the final equilibrium composition for the first assigned point (i.e., the combustion chamber for a rocket problem), then a small amount of computer time can be saved by using an INSERT card. The more important reason for the INSERT option is that, in rare instances, it is impossible to obtain convergence without the use of an

INSERT card. This occurs when, by considering gases only, the temperature becomes extremely low. When this happens, the program outputs the following message: "LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE BEEN INCLUDED ON AN INSERT CARD" and no solution will be obtained. The user should resubmit the problem with one or more appropriate condensed species listed on an INSERT card.

The use of ØMIT and INSERT cards is completely optional; however when used, each card must contain either the code word ØMIT in columns 1 to 4 or INSERT in columns 1 to 6 and the chemical formulas of from one to four product species. The names of the species must be left-adjusted and begin in columns 16, 31, 46, or 61. In addition, the species name must be punched on the card exactly as it appears in the THERMØ data. This means that the order of the chemical elements within the species name, the formula numbers, and the state of the species must all be identical. For example, gaseous ammonia would commonly appear as NH_3. Because of the alphabetizing scheme used for thermodynamic data, this species is written as H3N1(G).

4. NAMELISTS DATA

The word NAMELIST is a FØRTRAN IV statement and provides a convenient way of inputting data. One of the major advantages of the NAMELIST input method is that the data can be placed in any order and need not be placed within pre-specified card columns as is the case for the REACTANTS data. A secondary advantage is that the variable name appears with its numerical value on a card, thus making it easy to tell the purpose of each piece of data without having to refer to a program manual or to the program listing. Even though inputting data by means of NAMELIST is convenient, the following rules must be observed.

All data input by means of a NAMELIST statement must be associated with a NAMELIST name, and for this program there are only two: INPT2 and RKTINP. The first column of all NAMELIST data cards may not be used and must be blank. The second column of the first card only must contain a $ character. The applicable NAMELIST name must be placed on the first card only. The name must begin in column 3, and must be followed by at least one blank column.

Each NAMELIST name is assigned a group of FØRTRAN variables. (The variables belonging to INPT2 and RKTINP are listed in Tables V and VI, respectively.) These variables are assigned to a NAMELIST name within the program, and numeric data can only be input in conjunction with a NAMELIST name.

Although, in general, there are seven forms that input data may take, only three are of interest for this report. These are integer constants, real number constants, and logical constants. These are defined as follows:

a. An integer consists of one to eleven digits written without a decimal point.

b. A real number constant may be written in two ways. The first form is from one to nine digits, including a decimal point, followed by an exponent. The exponent is written as the letter E followed by a sign and a one or two digit integer. For example 12345. could be written as 1.2345E04 or .12345+5, etc. The second form is one to nine digits, including a decimal point, but not followed by an exponent.

c. A logical constant may be either true or false. There are two forms in which the constant may be written. These are either .TRUE. or T .FALSE. or F. The periods before and after the long forms are mandatory.

Logical constants may be associated only with logical variables. Integer constants may be associated with real variables and vice versa, and the proper conversion is made automatically by the computer. Note that when inputting data without a NAMELIST statement this conversion may cause difficulties and should only be used with great care.

On a NAMELIST card, each piece of data must be written in conjunction with its variable name (e.g., P = 100, or INDEX = 3, or PSIA = .TRUE., etc.). The equal sign is mandatory, and the data items must be separated by commas. If more than one card is required, the last item on each card, except for the last card, must be a constant followed by a comma. A variable name may not be the last item on the card. The end of a group of data is signaled by a $ character. This may be on the same card as that containing the NAMELIST name if only one card is used or may be on any succeeding card, but it may not be the first character on a succeeding card. Note that it is not necessary to completely fill a card with data before beginning a subsequent card. In fact, the user may want to put each piece of data on separate cards. This facilitates subsequent data changes. One final note, it is not necessary to input data for every variable contained in a NAMELIST; however, each variable has been assigned a value within the program, and this value is used unless superseded by input data. The assigned values for all NAMELIST variables in this program are included in Tables V and VI.

To illustrate the preceding instructions, the following paragraphs discuss the specific NAMELIST data required by this program, what each data bit does, and then some specific examples.

The INPT2 NAMELIST data must be used for all problems. The variables in the INPT2 NAMELIST are listed and defined in Table V along with the type and assigned value of each variable. The type of problem (one of either TP, HP, RKT, or DETN), at least one pressure (P), and the relative amounts of fuel and oxidizer (i.e., one of either EQRAT, OF, FPCT, or FA) are required for each problem. The other variables are either completely optional or may be required only if a particular problem type is requested.

The variable JANF is a flag to indicate which thermodynamic data polynomial should be used. JANF=0 designates a polynomial of the form $C_p=A_1+A_2T+A_3T^2+A_4T^3+A_5T^4$. This is the form used by the Lewis Research Center and is also the form the Armament Laboratory uses after converting the JANAF data.

The Lewis program is quite flexible in the type of problems it will consider or the thermodynamic variables which may be fixed. For gun propellant problems, it is most advantageous to assign the enthalpy and pressure which, in system nomenclature, constitutes an RKT problem.

a. RKT Problem

If RKT = .TRUE. or T, then a rocket problem is solved. A rocket problem is one for which the combustion takes place at an assigned enthalpy (REACTANTS cards) and assigned pressure (single value in the P variable), followed by an isentropic expansion. The combustion temperature, the thermodynamic properties and rocket performance are calculated for the chamber, the throat, and assigned exit points. The exit points desired are specified in the RKTINP namelist. If a temperature is assigned (T variable), then combustion will be assumed to occur at that temperature and not at the assigned enthalpy. The RKT problem type combines the H,S and T,S problems of the earlier program version. Note that, when this option is selected, the second set of NAMELIST data, RKTINP, is then required. The combustion gas conductivity and viscosity are computed for this option only.

b. DETN Problem

If DETN = .TRUE. or T, then the program solves a Chapman-Jouget detonation problem. The thermodynamic properties and composition downstream of the detonation wave are calculated for an assigned pressure and temperature upstream of the wave. This detonation calculation is primarily oriented for gas phase detonations. It is of limited utility for computation of detonations in solids, as the specific heat polynomial of the reactants must be on the data tape, which will not, in general, be the case for a typical solid explosive constituent ingredient.

c. P, PSIA, and MMHG Variables

The value P may be either the combustion pressure of a rocket engine (RKT problem) or a pressure at which composition and thermodynamic properties (TP or HP problem) are desired. Up to 26 values may be input, but only one is permitted for an RKT problem. The program assumes that the units of the pressures are in atmospheres unless either PSIA or MMHG are set true. If PSIA = .TRUE. or T then the pressure units are assumed to be in psia units. If MMHG = .TRUE. or T then the pressure units are assumed to be in millimeters of mercury. PSIA and MMHG may not both be set true in the same problem.

d. T Variable

Values for the T variable should be input only if TP is set true or if an assigned chamber temperature is desired for RKT problem. The temperature units must be degrees Kelvin.

e. EQRAT, ØF, FPCT, and FA Variables

The relative amounts of total fuel and total oxidizer may be expressed in one (and only one for each problem) of four ways. The mixture ratio (ØF) and percent fuel (FPCT) are self evident. The fuel-to-air weight ratio (FA) and equivalence ratio (EQRAT) are new to this version of the program and are not of use for gun propellant calculations.

f. IDEBUG Variable

If IDEBUG = .TRUE. or T then a printout of the intermediate calculation details is obtained. This is intended primarily as a debugging aid in the event there are problems. The output is extensive and is explained on page 34 of Reference 1.

g. IØNS Variable

If IØNS = .TRUE. or T then the program will consider ionized species. The earlier Lewis program version could not handle ionic species although provision was made in one of the subroutines for future consideration of ions. This capability is included in the newer program and thermodynamic data for ionized species are available as well as a sample problem which uses IØNS = T.

h. EQL, FRØZ, PCP, SUBAR, and SUPAR Variables

The five RKTINP variables (EQL, FRØZ, PCP, SUBAR, and SUPAR) in the RKTINP namelist are listed in Table VI. Of these, only PCP is required. The RKTINP namelist is required only if RKT is set true in the INPT2 namelist.

(1) PCP Variable

The value PCP is the ratio of the chamber pressure to the exit pressure. This is one of the independent variables (along with the entropy) for the nozzle portion of a rocket problem, and as such, at least one value must be input. As many as 22 values may be input; however, unlike the older program, values for the chamber and throat should not be input. Pressure ratios for the subsonic portion of the nozzle may be used. Values must be ordered so that the magnitudes increase monotonically.

(2) SUBAR and SUPAR Variables

Gun propellant performance at specific area ratios corresponding to a given gas velocity, either subsonic or supersonic, may be requested. Subsonic ratios are read as SUBAR and supersonic as SUPAR. When assigned area ratios are requested, the range of PCP values should be large enough to include the assigned area ratios. If the range is not large enough, extrapolation may be performed. SUBAR values should be ordered such that the values decrease and the SUPAR data should increase. Thirteen of each variable are permitted. Note that the use of this program feature is completely optional.

(3) EQL and FRØZ Variables

The program will calculate performance for both equilibrium and frozen expansions unless instructed otherwise. If EQL = .FALSE. or F then the equilibrium expansion is omitted and only frozen performance is calculated. If FRØZ = .FALSE. or F then the frozen expansion is omitted and only equilibrium performance is calculated.

TABLE V. VARIABLES IN INPT2 NAMELIST

Variable Name	Variable Type	Value (Unless Set Differently)	Definitions
JANF	Integer	1.	Thermodynamic data polynomial indicater
P	Real	0.	Assigned pressures
T	Real	0.	Assigned temperatures
EQRAT	Real	0.	Equivalence ratio
ØF	Real	0.	Oxidant-to-fuel weight ratio
FPCT	Real	0.	Percent fuel by weight
FA	Real	0.	Fuel-to-air weight ratio
TP	Logical	False	Assigned temperature and pressure problem
HP	Logical	False	Assigned enthalpy and pressure problem
RKT	Logical	False	Rocket problem
DETN	Logical	False	Detonation problem
PSIA	Logical	False	Assigned pressure-to be in psia units
MMHG	Logical	False	Assigned pressures in millimeter of mercury units
IØNS	Logical	False	Consider ionic species
IDEBUG	Logical	False	Print intermediate output

TABLE VI. VARIABLES IN RKTINP NAMELIST

Variable Name	Variable Type	Value Unless Set Differently	Definition
EQL	Logical	True	Gun propellant performance assuming equilibrium composition to be calculated
FRØZ	Logical	False	Gun propellant performance assuming frozen composition to be calculated
PCP	Real	0.	Ratio of chamber pressure to exit pressure
SUBAR	Real	0.	Subsonic area ratios
SUPAR	Real	0.	Supersonic area ratios

Table VII contains the input data for several propellant performance cases, and the output is listed on Tables VIII through XI. These cases are respectively M-10 (Case 100), M-9 (Case 101), an HMX-rubber propellant system (Case 102), and an RDX-triamino-guanidine nitrate formulation (Case 106). A comparison of these data with experimental or independent theoretical solutions gives the following results.

	Tv	Fp	γ	Mw
Case 100				
Lewis	3312	366,548	1.22	25.1
Experimental	3034	346,180	1.23	24.2
Case 101				
Lewis	3853	394,180	1.17	27.2
Experimental	3840	396,840	1.20	26.5
Case 102				
Lewis	2566	377,584	1.28	18.9
Other Theoretical	2545	373,000	(--)	18.9
Case 106				
Lewis	2637	390,870	1.29	18.8
Other Theoretical	2647	391,000	(--)	18.8

The input data (Table VII) are discussed in the program writeup except that no ØMIT or INSERT cards are used.

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TABLE VII. INPUT DATA FOR SAMPLE GUN PROPELLANT PROBLEMS

```
  3  1
C 24.0    H 29.5    O 41.3    N 10.6                 1.0   -643100.   298.    F
C 12.0    H 11.0    N 1.0                             .33    27600.   298.    O
C 2.0     H 14.0    O 6.0     N 4.0                   .67   -66300.   298.    O
 CASE 100      PROPELLANT IS M-10
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=98.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  4  1
C 24.0    H 29.5    O 41.3    N 10.6                 1.0   -643100.   298.    F
C 3.0     H 5.0     O 9.0     N 3.0                   .96   -85300.   298.    O
C 12.0    H 11.0    N 1.0     N 4.0                   .02    27600.   298.    O
C 3.0     H 14.0    O 6.0                             .02   -66300.   298.    O
 CASE 101      PROPELLANT IS M-9
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=58.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  2  1
C 4.0     H 8.0     O 8.0     N 8.0                  1.0    17900.   298.    O
C 7.0     H 11.0    O .2      N .02                  1.0    -5000.   298.    F
 CASE 102      PROPELLANT IS HMX RUBBER
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=15.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  3  1
C 4.0     H 8.0     O 8.0     N 8.0                  1.0    17900.   298.    O
C 7.0     H 11.0    O .2      N .02                   .88   -5000.   298.    F
TI1.0                                                 .12       0.   298.    F
 CASE 103      PROPELLANT IS HMX-RUBBER WITH TITANIUM ADDED
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=17.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
  4  1
C 2.0     H 5.0     O 1.0     N 3.0                   .83    22500.   298.    F
C 4.0     H 6.0     N 4.0                             .17    52400.   298.    F
C 3.0     H 6.0     O 6.0     N 6.0                   .60    14900.   298.    O
C 1.0     H 9.0     O 3.0     N 7.0                   .40   -11500.   298.    O
 CASE 106      PROPELLANT IS RDX-TAG NITRATE
 $INPT2    JANF=0,P(1)=5000.,RKT=.TRUE.,FPCT=16.,PSIA=.TRUE.$
 $RKTINP   PCP(1)=1.2,1.4,1.6,2.0,3.0,4.0,5.0,10.0,68.0,FROZ=.FALSE.$
```

TABLE VIII. OUTPUT FOR CASE 100, M-10 PROPELLANT

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 100 PROPELLANT IS M-10

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 24.00000	H 29.50000	O 41.30000	N 10.60000	1.00000	-643100.000		298.00	-0.0000
OXIDANT	C 12.00000	H 11.00000	N 1.00000		.33000	27600.000		298.00	-0.0000
OXIDANT	C 2.00000	H 14.00000	O 6.00000	N 4.00000	.67000	-66300.000		298.00	-0.0030

O/F= .0204 PERCENT FUEL= 98.0000 EQUIVALENCE RATIO= 1.5547 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.788	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	190.3	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	2713	2441	2625	2553	2491	2391	2217	2101	2015	1766	1227
H, CAL/G	-562.7	-681.0	-601.2	-632.7	-659.3	-702.4	-776.2	-825.3	-861.6	-965.0	-1189.2
S, CAL/(G)(K)	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442	2.2442
M, MOL WT	25.125	25.137	25.130	25.133	25.135	25.138	25.141	25.143	25.143	25.144	25.148
(DLV/DLP)T	-1.00052	-1.00022	-1.00040	-1.00032	-1.00026	-1.00019	-1.00010	-1.00007	-1.00005	-1.00003	-1.00030
(DLV/DLT)P	1.0096	1.0040	1.0074	1.0058	1.0047	1.0033	1.0017	1.0010	1.0007	1.0003	1.0037
CP, CAL/(G)(K)	.4447	.4313	.4398	.4362	.4334	.4294	.4239	.4209	.4191	.4152	.4239
GAMMA (S)	1.2206	1.2263	1.2226	1.2241	1.2253	1.2272	1.2300	1.2316	1.2328	1.2352	1.2307
SON VEL,M/SEC	1046.8	995.0	1030.5	1016.7	1004.8	985.1	949.7	925.1	906.2	849.4	786.6
MACH NUMBER	0.000	1.000	.551	.753	.895	1.098	1.408	1.683	1.745	2.160	3.240
VEL, FT/SEC	0.0	3264.4	1861.8	2511.7	2950.7	3547.5	4385.6	4863.7	5188.8	6819.9	7512.1
VISC, G/CM-SEC	.000795	.000738	.000777	.000762	.000749	.000727	.000690	.000665	.000646	.000591	.000468
C, CAL/G-SEC-K	.000300	.000281	.000294	.000289	.000285	.000278	.000266	.000256	.000251	.000234	.000281
T, CV, DEG K	3312										
IMPETUS	366548.										
CSTAR, FT/SEC		4760	4760	4760	4760	4760	4760	4760	4760	4760	4760
CF		.686	.391	.528	.620	.745	.921	1.022	1.090	1.265	1.578
AE/AT		1.000	1.266	1.865	1.011	1.008	1.134	1.292	1.452	2.194	8.385
IVAC,LB-SEC/LB		184.2	213.9	190.5	185.1	184.8	192.3	199.0	204.2	219.6	251.5
I, LB-SEC/LB		101.5	57.9	78.1	91.7	110.3	136.3	151.2	161.3	187.1	233.5

TABLE VIII. Concluded

MOLE FRACTIONS

CH4	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	[illegible]
CO	.40188	.39739	.40060	.39943	.39834	.39637	.39229	.38896	.38611	.37565	.33827
CO2	.13746	.14230	.13888	.14019	.14130	.14335	[illegible]	.15091	.15378	.16431	.20966
H	.00104	.00046	.00082	.00066	.00054	.00039	.00020	.00012	.00000	.00002	.00000
HCN	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00000	.00000	.00000	.00000
HCO	.00016	.00006	.00013	.00011	.00009	.00007	.00004	.00002	.00002	.00001	.00000
H2	.10392	.10863	.10535	.10664	.10781	.10990	.11415	.11755	.12044	.13101	.17615
H2O	.23507	.23088	.23392	.23283	.23180	.22989	.22585	.22253	.21968	.20916	.16394
NH3	.00003	.00003	.00003	.00003	.00003	.00003	.00002	.00002	.00002	.00002	.00002
NO	.00005	.00001	.00004	.00002	.00002	.00001	.00000	.00000	.00000	.00000	0.00000
N2	.11974	.11983	.11978	.11980	.11982	.11984	.11986	.11987	.11987	.11987	.11989
OH	.00061	.00019	.00043	.00032	.00024	.00015	.00006	.00003	.00001	.00000	0.00000

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	C(S)	CH	CH2	CH3	CN	CH2	C2	C2N	C2H2
C2H4	C2N	C2N2	C2O	C3	HO2	H2O(L)	H2O(S)	N	NH
NH2	NO2	N2C	N2H4	N2O	N2O4	O	O2		

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

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 99.8 PERCENT OF GAS MIXTURE

TABLE IX. OUTPUT FOR CASE 101, M-9 PROPELLANT

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 101 PROPELLANT IS M-9

CHEMICAL FORMULA					WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 24.00000	H 29.50000	O 41.30000	N 10.60000	1.00000	-643100.000		298.00	-0.0000
OXIDANT	C 3.00000	H 5.00000	O 9.00000	N 3.00000	.96000	-85300.000		298.00	-0.0000
OXIDANT	C 12.00000	H 11.00000	N 1.00000	N 4.00000	.02000	27660.000		298.00	-0.0000
OXIDANT	C 3.00000	H 14.00000	O 6.00000		.02000	-66300.000		298.00	-0.0000

O/F= .7241 PERCENT FUEL= 58.0000 EQUIVALENCE RATIO= 1.3101 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.759	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	193.4	283.5	243.0	212.6	170.1	113.4	85.06	66.05	34.02	5.003
T, CP, DEG K	3298	3049	3217	3149	3091	2992	2815	2690	2594	2310	1648
H, CAL/G	-485.1	-615.8	-528.5	-564.3	-594.6	-644.0	-729.4	-786.8	-829.5	-952.5	-1224.6
S, CAL/(G)(K)	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389	2.2389
M, MOL WT	27.185	27.319	27.234	27.271	27.300	27.342	27.398	27.426	27.441	27.466	27.477
(DLV/DLP)T	-1.00614	-1.00326	-1.00508	-1.00429	-1.00366	-1.00276	-1.00157	-1.00101	-1.00070	-1.00021	-1.00001
(DLV/DLT)P	1.1238	1.0700	1.1051	1.0904	1.0786	1.0611	1.0364	1.0242	1.0173	1.0055	1.0001
CP, CAL/(G)(K)	.6142	.5393	.5888	.5680	.5509	.5245	.4849	.4636	.4507	.4253	.4038
GAMMA (S)	1.1685	1.1784	1.1713	1.1740	1.1765	1.1818	1.1892	1.1947	1.1985	1.2074	1.2163
SON VEL,M/SEC	1065.6	1045.7	1072.6	1061.7	1052.3	1036.6	1007.3	987.0	970.6	918.8	779.5
MACH NUMBER	0.000	1.000	.562	.767	.910	1.112	1.419	1.610	1.749	2.152	3.191
VEL, FT/SEC	0.0	3430.7	1976.6	2670.2	3140.5	3782.7	4691.1	5213.1	5569.8	6488.1	8161.4
VISC, G/CM-SEC	.000906	.000866	.000895	.000884	.000874	.000856	.000824	.000799	.000779	.000719	.000572
C, CAL/G-SEC-K	.000291	.000278	.000287	.000283	.000280	.000274	.000265	.000257	.000252	.000235	.000195
T, CV, DEG K	3353										
IMPETUS	394 [illegible]										
CSTAR, FT/SEC		5121	5121	5121	5121	5121	5121	5121	5121	5121	5121
CF		.670	.386	.521	.613	.739	.916	1.018	1.088	1.267	1.594
AE/AT		1.003	1.253	1.058	1.006	1.011	1.148	1.315	1.483	2.265	8.734
IVAC,LB-SEC/LB		197.1	227.7	203.3	197.9	198.0	206.7	214.4	228.3	237.7	274.1
I, LB-SEC/LB		106.6	61.4	83.0	97.6	117.6	145.8	162.0	173.1	201.7	253.7

TABLE IX. Concluded

MOLE FRACTIONS

CO	.27808	.27371	.27656	.27535	.27438	.27285	.27035	.26867	.26735	.26277	.24173
CO2	.21989	.22997	.22194	.22344	.22496	.22727	.23084	.23583	.23463	.23969	.26894
H	.00427	.00288	.00380	.00342	.00318	.00260	.00180	.00134	.00104	.00042	.00001
HCO	.00016	.00009	.00013	.00012	.00010	.00006	.00005	.00004	.00003	.00001	.00000
HO2	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	0.00000	0.00000
H2	.04746	.04847	.04769	.04795	.04824	.04883	.05026	.05156	.05272	.05721	.07039
H2O	.28839	.29217	.28987	.29093	.29170	.29268	.29347	.29338	.29279	.28943	.26877
NH2	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	0.00000
NH3	.00001	.00001	.00001	.00001	.00001	.00000	.00000	.00000	.00000	.00000	.00000
NO	.00243	.00116	.00195	.00160	.00133	.00095	.00048	.00027	.00017	.00003	.00000
N2	.14733	.14870	.14784	.14822	.14851	.14693	.14948	.14973	.14987	.15008	.15015
O	.00258	.00022	.00044	.00034	.00026	.00017	.00007	.00003	.00002	.00000	0.00000
OH	.01079	.00607	.00911	.00780	.00676	.00521	.00303	.00195	.00134	.00034	.00000
O2	.00140	.00054	.00106	.00092	.00064	.00041	.00016	.00008	.00004	.00000	0.00000

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	C(S)	CH	CH2	CH3	CH4	CN	CN2	C2	C2H
C2H2	C2H4	C2N	C2N2	C2O	C3	HCN	H2O(L)	H2O(S)	N
NH	NO2	N2C	N2H4	N2O	N2O4				

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

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 98.0 PERCENT OF GAS MIXTURE

TABLE X. OUTPUT FOR CASE 102, HMX-RUBBER

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 102 PROPELLANT IS HMX-RUBBER

	CHEMICAL FORMULA				WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
OXIDANT	C 4.00000	H 8.00000	O 8.00000	N 8.00000	1.00000	17900.000		298.00	-0.0000
FUEL	C 7.00000	H 11.00000	O .20000	N .02000	1.00000	-5800.000		298.00	-0.0000

O/F= 5.6667 PERCENT FUEL= 15.0000 EQUIVALENCE RATIO= 2.7550 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.819	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	187.0	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	1995	1758	1918	1856	1805	1724	1592	1510	1453	1310	1070
H, CAL/G	43.8	-73.8	6.3	-24.2	-49.8	-91.0	-160.9	-207.0	-241.0	-337.8	-557.9
S, CAL/(G)(K)	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686	2.4686
M, MOL WT	18.902	19.006	18.925	18.950	18.976	19.030	19.163	19.264	19.392	19.796	21.091
(DLV/DLP)T	-1.01474	-1.02159	-1.01644	-1.01815	-1.01982	-1.02299	-1.02975	-1.03507	-1.03932	-1.05817	-1.07938
(DLV/DLT)P	1.0946	1.1603	1.1127	1.1309	1.1489	1.1839	1.2631	1.3303	1.3876	1.7068	2.2465
CP, CAL/(G)(K)	.5308	.5951	.5452	.5607	.5769	.6103	.6929	.7693	.8383	1.3[illegible]12	2.3570
GAMMA (S)	1.2863	1.2791	1.2854	1.2837	1.2817	1.2769	1.2642	1.2531	1.2438	1.[illegible]303	1.1394
SON VEL, M/SEC	1062.5	991.7	1040.8	1022.5	1006.7	980.7	934.5	903.3	880.2	809.4	693.4
MACH NUMBER	0.000	1.000	.538	.738	.879	1.083	1.400	1.604	1.754	2.208	3.2[illegible]
VEL, FT/SEC	0.0	3253.6	1837.3	2474.8	2903.8	3484.2	4293.7	4752.8	5064.5	5862.5	7361.[illegible]
VISC, G/CM-SEC	.000604	.000555	.000588	.000576	.000565	.000548	.000521	.000504	.000493	.000469	.000416
C, CAL/G-SEC-K	.000391	.000357	.000380	.000371	.000364	.000351	.000331	.000317	.000307	.000285	.000249
T, CV, DEG K	2566										
IMPETUS	377584.										
CSTAR, FT/SEC		4627	4627	4627	4627	4627	4627	4627	4627	4627	4627
CF		.703	.397	.535	.628	.753	.928	1.027	1.095	1.267	1.591
AE/AT		1.000	1.259	1.072	1.014	1.008	1.123	1.279	1.431	2.184	9.087
IVAC, LB-SEC/LB		180.2	210.6	187.0	181.4	180.6	187.3	193.6	198.6	213.6	248.0
I, LB-SEC/LB		101.1	57.1	76.9	90.3	108.3	133.5	147.7	157.4	182.2	228.8

TABLE X. Concluded

MOLE FRACTIONS

C(S)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	.00998	.07542
CH3	.00003	.00001	.00002	.00002	.00001	.00001	.00000	.00000	.00000	.00000	.00000
CH4	.00418	.00735	.00494	.00571	.00649	.00805	.01175	.01508	.01803	.02372	.02120
CO	.40882	.40490	.40640	.40595	.40546	.40443	.40181	.39928	.39691	.37715	.27309
CO2	.00566	.00741	.00608	.00650	.00693	.00780	.00992	.01194	.01383	.02277	.06092
C2H2	.00002	.00001	.00002	.00001	.00001	.00001	.00000	.00000	.00000	.00000	0.00000
C2H4	.00002	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00000
H	.00005	.00001	.00003	.00002	.00001	.00001	.00000	.00000	.00000	.00000	0.00000
HCN	.00136	.00074	.00114	.00098	.00085	.00067	.00043	.00030	.00023	.00009	.00001
HCO	.00007	.00002	.00005	.00004	.00003	.00002	.00001	.00000	.00000	.00000	.00000
H2	.34336	.33876	.34237	.34127	.34009	.33764	.33162	.32618	.32141	.30765	.28640
H2O	.02153	.02240	.02165	.02185	.02210	.02266	.02413	.02545	.02656	.03329	.05793
NH3	.00065	.00056	.00062	.00060	.00057	.00054	.00049	.00045	.00042	.00033	.00015
N2	.21627	.21782	.21600	.21704	.21742	.21814	.21982	.22129	.22259	.22510	.22400

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CN	CN2	C2	C2H	C2N	C2N2	C2O
C3	HO2	H2O(L)	H2O(S)	N	NH	NH2	NO	NO2	N2O
N2H4	N2O	N2O4	O	OH	O2				

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

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 99.4 PERCENT OF GAS MIXTURE

TABLE XI. OUTPUT FOR CASE 106, RDX-TRIAMINO GUANIDINE NITRATE

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

PC = 5000.0 PSIA

CASE 106 PROPELLANT IS RDX-TAG NITRATE

	CHEMICAL FORMULA								WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	C 2.00000	H 5.00000	O 1.00000	N 3.00000					.83000	22500.000		298.00	-0.0000
FUEL	C 4.00000	H 6.00000	N 4.00000						.17000	52400.000		298.00	-0.0000
OXIDANT	C 3.00000	H 6.00000	O 6.00000	N 6.00000					.60000	14900.000		298.00	-0.0000
OXIDANT	C 1.00000	H 9.00000	O 3.00000	N 7.00000					.40000	-11500.000		298.00	-0.0000

O/F= 2.3333 PERCENT FUEL= 30.0000 EQUIVALENCE RATIO= 2.6826 DENSITY= 0.0000

	CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
PC/P	1.000	1.826	1.200	1.400	1.600	2.000	3.000	4.000	5.000	10.000	68.000
P, ATM	340.2	186.4	283.5	243.0	212.6	170.1	113.4	85.06	68.05	34.02	5.003
T, CP, DEG K	2051	1795	1970	1904	1848	1759	1610	1517	1451	1285	1019
H, CAL/G	[illegible]	-24.9	58.7	27.1	.6	-42.0	-114.2	-161.6	-196.4	-294.	-513.2
S, CAL/(G)(K)	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166	2.5166
M, MOL WT	18.760	18.777	18.763	18.766	18.77	18.783	18.823	18.875	18.934	19.227	20.449
(DLV/DLP)T	-1.00316	-1.00507	-1.00350	-1.00393	-1.00443	-1.00561	-1.00943	-1.01395	-1.01859	-1.03637	-1.07293
(DLV/DLT)P	1.0171	1.0359	1.0207	1.0249	1.0297	1.0412	1.0794	1.1274	1.1795	1.4046	2.1373
CP, CAL/(G)(K)	.4866	.4956	.4871	.4887	.4914	.4995	.5338	.5833	.6413	.9227	2.2581
GAMMA (S)	1.2855	1.2888	1.2871	1.2881	1.2886	1.2886	1.2837	1.2746	1.2644	1.2264	1.1412
SON VEL,M/SEC	1081.0	1012.0	1063.0	1042.3	1027.0	1001.7	9[illegible]5.6	922.7	897.5	825.6	687.6
MACH NUMBER	0.000	1.000	.538	.737	.877	1.079	1.393	1.596	1.747	2.195	3.288
VEL, FT/SEC	0.0	3320.3	1870.0	2518.8	2955.1	3545.2	4366.5	4838.7	5144.8	5944.9	7416.6
VISC, G/CM-SEC	.000624	.000568	.000606	.000592	.000580	.000561	.000528	.000508	.000493	.000460	.000397
L, CAL/G-SEC-K	.000401	.000366	.000390	.000381	.000374	.000361	.000340	.000326	.000316	.000289	.000234
T, CV, DEG K	2637										
IMPETUS	390870.										
CSTAR, FT/SEC		4704	4704	4704	4704	4704	4704	4704	4704	4704	4704
CF		.706	.398	.536	.627	.754	.928	1.027	1.094	1.264	1.577
AE/AT		1.000	1.282	1.073	1.014	1.005	1.118	1.266	1.417	2.139	8.693
IVAC,LB-SEC/LB		183.3	214.3	190.3	184.5	183.7	190.2	198.4	201.3	210.1	249.2
I, LB-SEC/LB		103.2	58.1	78.3	91.8	110.2	135.7	150.1	159.9	184.8	230.5

TABLE XI. Concluded

MOLE FRACTIONS

C(S)	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	.02182
CH3	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	0.00000
CH4	.00055	.00112	.00066	.00079	.00094	.00128	.00239	.00381	.00541	.01327	.03404
CO	.26713	.26459	.26649	.26587	.26527	.26408	.26121	.25841	.25569	.24392	.17825
CO2	.01182	.01421	.01244	.01304	.01360	.01466	.01708	.01927	.02130	.02960	.06425
H	.00007	.00001	.00005	.00003	.00002	.00001	.00000	.00000	.00000	.00000	0.00000
HCN	.00032	.00019	.00027	.00024	.00021	.00017	.00012	.00009	.00008	.00004	.00000
HCO	.00005	.00002	.00004	.00003	.00002	.00001	.00001	.00000	.00000	.00000	.00000
H2	.33571	.33705	.33618	.33654	.33682	.33717	.33707	.33598	.33431	.32430	.28869
H2O	.06992	.06806	.06938	.06890	.06848	.06777	.06659	.06602	.06582	.06659	.07784
NH3	.00069	.00061	.00066	.00064	.00062	.00060	.00057	.00055	.00054	.00047	.00024
N2	.31373	.31414	.31382	.31391	.31401	.31424	.31495	.31585	.31686	.32181	.33488

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CN	CN2	C2	C2H	C2H2	C2H4	C2N
C2N2	C2O	C3	HO2	H2O(L)	H2O(S)	N	NH	NH2	NO
NO2	N2O	N2H4	N2O	N2O4	O	OH	O2		

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

VISCOSITY AND CONDUCTIVITY VALUES BASED ON 99.8 PERCENT OF GAS MIXTURE

TABLE XII. THERMO DATA INPUT FORMAT FOR TITANIUM DIOXIDE

```
 -62000.0   9 51     TITANIUM DIOXIDE (TIO2) IDEAL GAS
298 300 400 500 600 700 800 9001000
 10.838  10.858  11.820  12.548  13.079  13.464  13.746  13.957  14.117
  0.000    .020   1.156   2.376   3.659   4.987   6.348   7.734   9.138
 56.146  56.213  59.474  62.194  64.531  66.578  68.395  70.027  71.506
1000110012001300140015001600170018001900200021002200230024002500260027002800290O
3000310032003300340035003600370038003900400041004200430044004500460047004800490O
5000510052005300540055005600570058005900600O
 14.117  14.[illegible]  14.339  14.417  14.480  14.532  14.575  14.611  14.641  14.667
 14.690  14.709  14.725  14.741  14.754  14.765  14.776  14.785  14.793  14.800
 14.807  14.813  14.819  14.824  14.828  14.832  14.836  14.840  14.843  14.846
 14.849  14.852  14.854  14.856  14.858  14.860  14.862  14.864  14.866  14.867
 14.869  14.870  14.871  14.872  14.874  14.875  14.876  14.877  14.878  14.878
 14.879
  9.138  10.556  11.985  13.423  14.868  16.319  17.774  [illegible]  20.696  22.162
 23.630  25.099  26.571  28.045  29.519  30.995  32.472  33.950  35.429  36.909
 38.389  39.870  41.352  42.834  44.317  45.800  47.283  48.767  50.251  51.736
 53.220  54.705  56.191  57.676  59.162  60.648  62.134  63.620  65.107  66.593
 68.080  69.567  71.054  72.541  74.029  75.516  77.004  78.491  79.979  81.467
 82.955
 71.506  72.858  74.101  75.252  76.323  77.324  78.263  79.147  79.948  80.776
 81.529  82.246  82.931  83.586  84.213  84.816  85.395  85.953  86.491  87.010
 87.512  87.997  88.468  88.924  89.336  89.796  90.214  90.621  91.017  91.402
 91.778  92.145  92.503  92.852  93.194  93.528  93.854  94.174  94.487  94.794
 95.094  95.388  95.677  95.960  96.238  96.511  96.779  97.043  97.301  97.556
 97.806
```

TABLE XIII. THERMØ DATA OUTPUT FORMAT FOR TITANIUM DIOXIDE

TITANIUM DIOXIDE (TIO2) IDEAL GAS

HO = -62000.0

VALUES OF G
COEFFICIENTS ARE
~~.30725340E+01 .10003020E-01 -.11120307E-34 .49403359E-08 -.67934354E-12 -.32500921E+05 .79567663E+01~~
-.33589155E-02 -.54917462E-02 -.15152376E-01

T	CP	CCP	HT	CHT	ST	CST	DCP	DHT	DST
298.	10.838	10.838	0.000	0.000	56.146	56.146	.006	0.000	.000
~~300.~~	~~10.850~~	~~10.866~~	~~.020~~	~~.022~~	~~56.213~~	~~56.219~~	~~.002~~	.002	.006
400.	11.820	11.816	1.156	1.158	59.474	59.480	.004	.002	.006
500.	12.548	12.540	2.376	2.377	62.194	62.198	.008	.001	.004
600.	13.079	13.076	3.659	3.659	64.531	64.534	.003	.000	.003
700.	13.464	13.465	4.987	4.987	66.578	66.581	.001	.000	.003
800.	13.746	13.746	6.348	6.349	68.395	68.398	.000	.001	.003
~~900.~~	~~13.957~~	~~13.953~~	~~7.734~~	~~7.734~~	~~70.027~~	~~70.030~~	.004	.000	.002
1000.	14.117	14.118	9.138	9.138	71.506	71.509	.001	.000	.003

VALUES OF G
COEFFICIENTS ARE
.62406076E+01 .12046967E-02 -.50184624E-06 .85525393E-10 -.53125222E-14 -.32336518E+05 -.81070897E+01
.95768211E-01 .22837632E-01 .10773479E+00

T	CP	CCP	HT	CHT	ST	CST	DCP	DHT	DST
1000.	14.117	14.117	9.138	9.138	71.506	71.506	.000	.000	.000
1100.	14.241	14.214	10.556	10.555	72.858	72.856	.027	.001	.002
1200.	14.339	14.301	11.985	11.981	74.101	74.097	.038	.004	.004
~~1300.~~	~~14.417~~	~~14.379~~	~~13.423~~	~~13.415~~	~~75.252~~	~~75.245~~	~~.038~~	~~.008~~	~~.007~~
1400.	14.480	14.447	14.868	14.856	76.323	76.313	.033	.012	.010
1500.	14.532	14.508	16.319	16.304	77.324	77.312	.024	.015	.012
1600.	14.575	14.561	17.774	17.757	78.263	78.250	.014	.017	.013
1700.	14.611	14.607	19.234	19.216	79.147	79.134	.004	.018	.013
1800.	14.641	14.646	20.696	20.678	79.948	79.970	.005	.018	.022
~~1900.~~	~~14.667~~	~~14.681~~	~~22.162~~	~~22.145~~	~~80.776~~	~~80.763~~	~~.014~~	~~.017~~	~~.013~~
2000.	14.690	14.709	23.630	23.614	81.529	81.516	.019	.016	.013
2100.	14.709	14.734	25.099	25.086	82.246	82.235	.025	.013	.011
2200.	14.726	14.754	26.571	26.561	82.931	82.921	.028	.010	.010
2300.	14.741	14.771	28.045	28.037	83.586	83.577	.030	.008	.009
2400.	14.754	14.784	29.519	29.515	84.213	84.206	.030	.004	.007
~~2500.~~	~~14.766~~	~~14.796~~	~~30.995~~	~~30.994~~	~~84.816~~	~~84.809~~	~~.030~~	~~.001~~	~~.007~~
2600.	14.776	14.803	32.472	32.474	85.395	85.390	.027	.002	.005
2700.	14.785	14.809	33.950	33.954	85.953	85.949	.024	.004	.004
2800.	14.793	14.814	35.429	35.435	86.491	86.487	.021	.006	.004
2900.	14.800	14.817	36.909	36.917	87.010	87.007	.017	.008	.003
3000.	14.807	14.819	38.389	38.399	87.512	87.510	.012	.010	.002
~~3100.~~	~~14.813~~	~~14.821~~	~~39.870~~	~~39.881~~	~~87.997~~	~~87.995~~	~~.008~~	~~.011~~	~~.002~~
3200.	14.819	14.821	41.352	41.363	88.468	88.466	.002	.011	.002
3300.	14.824	14.822	42.834	42.845	88.924	88.922	.002	.011	.002
3400.	14.828	14.823	44.317	44.327	89.336	89.365	.005	.010	.029
3500.	14.832	14.823	45.800	45.810	89.796	89.794	.009	.010	.002
3600.	14.836	14.824	47.283	47.292	90.214	90.212	.012	.009	.002
~~3700.~~	~~14.840~~	~~14.825~~	~~48.767~~	~~48.775~~	~~90.621~~	~~90.618~~	~~.015~~	~~.008~~	~~.003~~
3800.	14.843	14.827	50.251	[illegible].257	91.017	91.013	.016	.006	.004
3900.	14.846	14.829	51.736	[illegible]	91.402	91.399	.017	.004	.003
4000.	14.849	14.832	53.220	53.[illegible]	91.778	91.774	.017	.003	.004
4100.	14.852	14.836	54.705	54.706	92.145	92.140	.017	.001	.005
4200.	14.854	14.839	56.191	56.190	92.503	92.498	.015	.001	.005
4300.	14.856	14.844	57.676	57.674	92.852	92.847	.012	.002	.005
4400.	14.858	14.848	59.162	59.159	93.194	93.188	.010	.003	.006
4500.	14.860	14.854	60.643	60.644	93.528	93.522	.006	.00'	.006
4600.	14.862	14.859	62.134	62.130	93.854	93.849	.003	.004	.005
4700.	14.864	14.865	63.620	63.616	94.174	94.168	.001	.004	.006
4800.	14.866	14.871	65.107	65.103	94.487	94.481	.005	.004	.006
~~4900.~~	~~14.867~~	~~14.876~~	~~66.593~~	~~66.590~~	~~94.794~~	~~94.788~~	~~.009~~	~~.003~~	~~.006~~
5000.	14.869	14.881	68.080	68.078	95.094	95.089	.012	.002	.005
5100.	14.870	14.886	69.567	69.566	95.388	95.383	.016	.001	.005
5200.	14.871	14.889	71.054	71.055	95.677	95.672	.018	.001	.005
5300.	14.872	14.892	72.541	72.544	95.960	95.956	.020	.003	.004
5400.	14.874	14.893	74.029	74.033	96.238	96.235	.019	.004	.003
~~5500.~~	~~14.875~~	~~14.892~~	~~75.516~~	~~75.523~~	~~96.511~~	~~96.508~~	~~.017~~	~~.007~~	~~.003~~
5600.	14.876	14.889	77.004	77.012	96.779	96.776	.013	.008	.003
5700.	14.877	14.883	78.491	78.500	97.043	97.040	.006	.009	.003
5800.	14.878	14.875	79.979	79.988	97.301	97.298	.003	.009	.003
5900.	14.878	14.862	81.467	81.475	97.556	97.553	.016	.008	.003
6000.	14.879	14.847	82.955	82.960	97.806	97.802	.032	.005	.004

TABLE XIV. DATA TAPE FORM FOR THERMØ DATA OUTPUT

```
TIO2                J 6/70TI  10   200  000  06  298.000  6000.000          1
 0.62406876E+01 0.12846967E-02-0.50184624E-06 0.85525393E-10-0.53125222E-14    2
-0.33336518E+05-0.81878897E+01 0.30725348E+01 0.10883020E-01-0.11120307E-04    3
 0.49483359E-08-0.67934354E-12-0.32508921E+05 0.79567663E+01                   4
```

SECTION V

THERMØ DATA PROGRAM

The program (Appendix II) to fit the tabular JANAF thermochemical data to the Lewis polynomial is relatively simple and straightfor ard. JANAF data for Cp, H, and S is read in the tabular form for two temperature ranges 298° to 1,000°K and 1,000° to 6,000°K. The format is as shown in Table XII for the gas TIØ2. The first line consists of the reference heat of formation to 298°K in calories per mole, the number of points in the first temperature range and the number of points in the second temperature range, followed by a species identifier. The tabular temperature references for the first interval are then listed followed by the appropriate Cp, H, and S values. This sequence is then repeated for the second temperature range. Subsequent to data input, the program establishes a matrix which it solves by an inversion procedure to obtain the required polynomial constants. These constants are then output in the form suitable for inclusion on the Lewis program thermodynamic data tape.

The output is as shown on Table XIII for the $TiØ_2$ species which is also shown on the input. The coefficients required on the data card for the first temperature range are shown on the first line followed by a comparison between the tabular data and the generated polynomials for the three functions of interest. It can be seen that the data fit is quite good. These data are followed by the required constants for the second temperature range and a similar comparison of polynomial and tabular results.

These results are read onto the data tape in the form shown on Table XIV. There are four cards per species. The first line consists of the empirical formula in columns 1 to 12. A gaseous species has no subscript, a liquid, has subscript L, and a solid, has subscript S. Columns 19 to 21 contain a code for the data source, in this case, a J for the JANAF tables. Columns 22 to 24 are the month and year of polynomial computation. The first through the fourth atoms in the species are inserted in columns 25 and 26, 30 and 31, 35 and 36, 40 and 41, while the respective number of atoms are placed in columns 27 to 29, 32 to 34, 37 to 39, and 42 to 44. Column 45 is used for the phase of the species G, L, or S. Columns 46 through 55 have the lower temperature bound at which the species exists with the upper temperature bound being placed in columns 56 through 65.

Cards 2, 3, and 4 contain the 14 polynomial constants, five each on cards 2 and 3 and four on card 4.

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APPENDIX I

LEWIS PROGRAM LISTING

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```
      PROGRAM P1712(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE4,TAPE9)  P1712  00002
C                                                                       P1712  00003
C     I C R P G  REFERENCE PROGRAM  ODE                                 P1712  00004
C     DECK SEQUENCED BY SUBROUTINE                                      P1712  00005
C     THERMODYNAMIC DATA FOLLOWS SOURCE DECK                            P1712  00006
C     DATA FOR TEST CASES FOLLOWS THERMODYNAMIC DATA                    P1712  00007
C     PROGRAM USES TAPE UNIT 4 FOR THERMO DATA                          P1712  00008
C                                                                       P1712  00009
C     ODE  ICRPG REFERENCE PROGRAM                                      P1712  00010
C                                                                       P1712  00011
C  MAIN PROGRAM                                                         P1712  00012
C                                                                       P1712  00013
      DOUBLE PRECISION G,X                                              P1712  00014
      INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END,SUB            P1712  00015
      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT         P1712  00016
      LOGICAL SHOCK,MHHG,PASCAL,EV,IC,DETN,CPCVFR,CPCVEQ,SIUNIT,EUNITS  P1712  00017
C                                                                       P1712  00018
      DIMENSION OMIT(3,3),NOD(4),ENSERT(3,3),LH(2),LVP(2) ,LVM(2)       P1712  00019
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712  00020
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)  P1712  00021
     2  ,TOTN(13)                                                       P1712  00022
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  00023
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  00024
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712  00025
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  00026
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  00027
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00028
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  00029
      COMMON /DOUBLE/ G(20,21), X(20)                                   P1712  00030
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  00031
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  00032
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  00033
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  00034
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0                             P1712  00035
C                                                                       P1712  00036
      EQUIVALENCE (OMIT,ENLN),(ENSERT,EN(1,3))                          P1712  00037
C                                                                       P1712  00038
      DATA MIT/4HOMIT/,BLANK/1H /, PSIA/4HPSIA/,REAC/4HREAC/,           P1712  00039
     1   INPUT/4HINPU/,IE/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/   P1712  00040
      DATA LH/4HH,CA,4HL/G /,LVP/2HV+,1H /,LVM/2HV-,1H /,NMLT/4HNAME/   P1712  00041
C                                                                       P1712  00042
      NAMELIST/INPT2/JANF,P,T,EQRAT,OF,FPCT,FA,TP,HP,SP,RKT             P1712  00043
     1,PSIA,MHHG,SHOCK,IONS,EV,V,DETN,CPCVFR,CPCVEQ,IDEBUG              P1712  00044
     2,SIUNIT,EUNITS                                                    P1712  00045
C                                                                       P1712  00046
      TLOW = 0.                                                         P1712  00047
      NEWR = .FALSE.                                                    P1712  00048
      DO 399 I=1,15                                                     P1712  00049
      DO 398 J=1,150                                                    P1712  00050
      A(I,J) = 0.0                                                      P1712  00051
  398 CONTINUE                                                          P1712  00052
  399 CONTINUE                                                          P1712  00053
C                                                                       P1712  00054
```

```
      1 WRITE(6,400)                                                       P1712 00055
  400 FORMAT(1H1)                                                          P1712 00056
      READ(5,1204) NREAC,NCASE,NSRT,NMIT                                   P1712 00057
 1204 FORMAT(4I3)                                                          P1712 00058
      IF(NREAC.LE.0.OR.NCASE.LE.0) WRITE(6,1023) NREAC,NCASE               P1712 00059
 1023 FORMAT(1H ,*NO REACTANTS OR NO CASES SPECIFIED ON TYPE 1 DATA CARD P1712 00060
     1, NREAC =*,I3,*  NCASE=*,I3)                                         P1712 00061
   11 NOMIT = 0                                                            P1712 00062
      NSERT = 0                                                            P1712 00063
      MOLES = .FALSE.                                                      P1712 00064
      CALL REACT                                                           P1712 00065
      IF(L.EQ.0)  WRITE(6,52)                                              P1712 00066
   52 FORMAT(24H ERROR IN REACTANT CARDS)                                  P1712 00067
C                                                                          P1712 00068
C     CHECK INSERT CARDS                                                   P1712 00069
C                                                                          P1712 00070
      IF(NSRT.LE.0) GO TO 205                                              P1712 00071
  180 DO 185 K=1,NSRT                                                      P1712 00072
      READ(5,204) (DATA(J),J=1,15)                                         P1712 00073
      WRITE(6,2045) (DATA(J),J=1,15)                                       P1712 00074
  204 FORMAT(5(3A4,3X))                                                    P1712 00075
 2045 FORMAT(1X,5(3A4,3X))                                                 P1712 00076
      DO 185 I=1,15,3                                                      P1712 00077
      IF (DATA(I).EQ.BLANK) GO TO 185                                      P1712 00078
      NSERT = NSERT+1                                                      P1712 00079
      ENSERT(1,NSERT) = DATA(I)                                            P1712 00080
      ENSERT(2,NSERT) = DATA(I+1)                                          P1712 00081
      ENSERT(3,NSERT) = DATA(I+2)                                          P1712 00082
  185 CONTINUE                                                             P1712 00083
C                                                                          P1712 00084
C     CHECK OMIT CARDS                                                     P1712 00085
C                                                                          P1712 00086
  205 IF(NMIT.LE.0) GO TO 210                                              P1712 00087
      DO 208 K=1,NMIT                                                      P1712 00088
      READ(5,204) (DATA(J),J=1,15)                                         P1712 00089
      WRITE(6,2045) (DATA(J),J=1,15)                                       P1712 00090
      DO 208 I=1,15,3                                                      P1712 00091
      IF(DATA(I).EQ.BLANK) GO TO 208                                       P1712 00092
      NOMIT = NOMIT+1                                                      P1712 00093
      OMIT(1,NOMIT) = DATA(I)                                              P1712 00094
      OMIT(2,NOMIT) = DATA(I+1)                                            P1712 00095
      OMIT(3,NOMIT) = DATA(I+2)                                            P1712 00096
  208 CONTINUE                                                             P1712 00097
      NEWR= .TRUE.                                                         P1712 00098
C                                                                          P1712 00099
C     BEGIN NAMELIST INPT2                                                 P1712 00100
C                                                                          P1712 00101
  210 DO 500 NCS=1,NCASE                                                   P1712 00102
      DO 300 I=1,26                                                        P1712 00103
      OCP(I) = 0.                                                          P1712 00104
      P(I)= 0.                                                             P1712 00105
      T(I)= 0.                                                             P1712 00106
      V(I) = 0.                                                            P1712 00107
```

```
  300 CONTINUE                                                    P1712   00108
      V1 = 0.                                                     P1712   00109
      V2 = 0.                                                     P1712   00110
      RHOP = 0.                                                   P1712   00111
      KASE= 0                                                     P1712   00112
      TP = .FALSE.                                                P1712   00113
      HP=.FALSE.                                                  P1712   00114
      SP=.FALSE.                                                  P1712   00115
      RKT = .FALSE.                                               P1712   00116
      CPCVFR = .FALSE.                                            P1712   00117
      CPCVEQ = .FALSE.                                            P1712   00118
      SHOCK = .FALSE.                                             P1712   00119
      DETN = .FALSE.                                              P1712   00120
      EV = .FALSE.                                                P1712   00121
      PASCAL = .FALSE.                                            P1712   00122
      MMHG   = .FALSE.                                            P1712   00123
      PSIA = .FALSE.                                              P1712   00124
      R = 1.987165                                                P1712   00125
      RR = 4184.*R                                                P1712   00126
      SIUNIT = .FALSE.                                            P1712   00127
      EUNITS = .FALSE.                                            P1712   00128
      IONS = .FALSE.                                              P1712   00129
      IDEBUG=.FALSE.                                              P1712   00130
      FA = 0.                                                     P1712   00131
      OF = 0.                                                     P1712   00132
      EQRAT= 0.                                                   P1712   00133
      FPCT= 0.                                                    P1712   00134
      ECL = .TRUE.                                                P1712   00135
      READ(5,303)KASE                                             P1712   00136
  303 FORMAT(13A6,A2)                                             P1712   00137
      READ(5,INPT2)                                               P1712   00138
      DO 305 I=1,26                                               P1712   00139
      IF(P(I ).EQ.0.) GO TO 322                                   P1712   00140
      NP = I                                                      P1712   00141
      IF (MMHG) P(NP) = P(NP)/760.                                P1712   00142
      IF (PASCAL) P(NP) = P(NP)/101325.                           P1712   00143
      IF(PSIA        )  P(NP)=P(NP)/14.696006                     P1712   00144
  305 CONTINUE                                                    P1712   00145
  322 IF (FA.NE.0.) OF = 1./FA                                    P1712   00146
      IF(EQRAT.EQ.0.) GO TO 725                                   P1712   00147
      OF= (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))        P1712   00148
      GO TO 727                                                   P1712   00149
  725 IF(OF.NE.0.) GO TO 727                                      P1712   00150
      IF(FPCT.EQ.0.) GO TO 9051                                   P1712   00151
      OF= (100.-FPCT)/FPCT                                        P1712   00152
      GO TO 727                                                   P1712   00153
 9051 WRITE(6,724)                                                P1712   00154
  724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT  )  P1712   00155
      IF(WP(2).NE.1.) OF=WP(1)/WP(2)                              P1712   00156
  727 WP(1) = OF                                                  P1712   00157
      WP(2) = 1.                                                  P1712   00158
      SUM = WP(1)+WP(2)                                           P1712   00159
      FPCT = 100.*WP(2)/SUM                                       P1712   00160
```

```
      IF (EGRAT.NE.0.)  GO TO 746
      V2 = (WP(1)*VMIN(1)+WP(2)*VMIN(2))/SUM
      V1 = (WP(1)*VPLS(1)+WP(2)*VPLS(2))/SUM
      IF(V2.NE.0.)  EGRAT=ABS(V1/V2)
  746 DO 747 I=1,L
      BO(I) = (WP(1)*BOP(I,1)+WP(2)*BOP(I,2))/SUM
  747 CONTINUE
      IF (EGRAT.EQ.1.)  EGRAT= 1.000005
      IF(.NOT.IONS.OR.LMNT(L).EQ.IE)  GO TO 748
      L = L+1
      LLMT(L) = IE
      BO(L) = 0.
  748 HSUBO = (WP(1)*HPP(1)+WP(2)*HPP(2))/SUM
      WRITE (6,INPT2)
      WRITE(6,752)KASE
  752 FORMAT(1H0,13A6,A2/)
      WRITE (6,770)
  770 FORMAT (1H0,17X,4HFUEL ,13X,7HOXIDANT  ,12X,7HMIXTURE   //)
  780 FORMAT (1H 2A4,3E15.8/)
      WRITE (6,780) LH,HPP(2),HPP(1),HSUBO,LVP,VPLS(2),VPLS(1),V1,
     1LVM,VMIN(2),VMIN(1),V2
      HSUBO = HSUBO/R
      WRITE (6,785)
  785 FORMAT (8H ATOMS/G  )
      WRITE(6,780)(LLMT(I),BLANK,BOP(I,2),BOP(I,1),BO(I),I=1,L)
      RHOP = WP(2)*RHO(1)+WP(1)*RHO(2)
      IF(RHOP.NE.0.)  RHOP = (WP(1)+WP(2))*RHO(1)*RHO(2)/RHOP
  786 IF(NEWR) CALL SEARCH
      IQ1= L+1
      IF(NC.EQ.0)  GO TO 790
      DO 302 J=1,NS
      IF(IUSE(J).EQ.0) GO TO 302
      IF(IUSE(J).GT.0) IUSE(J)= -IUSE(J)
      IF(NSERT.EQ.0) GO TO 302
      DO 301 I=1,NSERT
      IF(SUB(J,1).NE.ENSERT(1,I)) GO TO 301
      IF(SUB(J,2).NE.ENSERT(2,I)) GO TO 301
      IF(SUB(J,3).NE.ENSERT(3,I)) GO TO 301
      ENSERT(1,I) =0.
      IQ1= IQ1+1
      IUSE(J)= -IUSE(J)
  301 CONTINUE
  302 CONTINUE
      NSERT = 0
  790 ITN= 35
      IC = .FALSE.
      PP = NS
      NPT = 1
      ENN = .1
      SUMN = ENN
      XI = NS - NC
      XI = ENN/XI
      XLN = ALOG(XI)
```

```
      DO 432 J=1,NS                              P1712   00214
      IF(IUSE(J).EQ.-10000)  IUSE(J)=0           P1712   00215
      EN(J,1) = 0.                               P1712   00216
      ENLN(J)=0.                                 P1712   00217
      IF (IUSE(J).NE.0)  GO TO 432               P1712   00218
      EN(J,1) = XI                               P1712   00219
      ENLN(J) = XLN                              P1712   00220
  432 CONTINUE                                   P1712   00221
      JSCL = 0                                   P1712   00222
      JLIQ = 0                                   P1712   00223
      IF(DETN) CALL DETON                        P1712   00224
      IF(RKT) CALL ROCKET                        P1712   00225
      IF (TP) CALL MOLIER                        P1712   00226
      IF(HP) CALL CMBSTN                         P1712   00227
  500 CONTINUE                                   P1712   00228
      GO TO 1                                    P1712   00229
      END                                        P1712   00230
```

```
      BLOCK DATA                                                        P1712  00231
C                                                                       P1712  00232
      DIMENSION ATEM(3,53)                                              P1712  00233
C                                                                       P1712  00234
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2)  P1712  00235
     1 ,TM,TLOW,TMIG,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  00236
     2 ,HPP(2),HMO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  00237
     3 ,ANUM(15,5),PECNT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00238
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  00239
      COMMON/OUPT/FMT(39),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)     P1712  00240
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),F4TI9,FA1,FA2         P1712  00241
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                        P1712  00242
C                                                                       P1712  00243
      EQUIVALENCE (ATOM(1,52),ATEM)                                     P1712  00244
C                                                                       P1712  00245
C ATOMIC SYMBOLS, WEIGHTS, AND VALENCES                                 P1712  00246
C                                                                       P1712  00247
      DATA ((ATOM(I,J),I=1,3),J=1,25)/                                  P1712  00248
     A    2HH , 1.008, 1.,   2HHE, 4.003, 0.,   2HLI, 6.940, 1.,        P1712  00249
     B    2HBE, 9.013, 2.,   2HB , 10.820, 3.,  2HC , 12.011, 4.,       P1712  00250
     C    2HN , 14.008, 0.,  2HO , 16.000,-2.,  2HF , 19.000,-1.,       P1712  00251
     D    2HNE, 20.183, 0.,  2HNA, 22.991, 1.,  2HMG, 24.320, 2.,       P1712  00252
     E    2HAL, 26.980, 3.,  2HSI, 28.090, 4.,  2HP , 30.975, 5.,       P1712  00253
     F    2HS , 32.066, 4.,  2HCL, 35.457,-1.,  2HAR, 39.944, 0.,       P1712  00254
     G    2HK , 39.100, 1.,  2HCA, 40.080, 2.,  2HSC, 44.960, 3.,       P1712  00255
     H    2HTI, 47.900, 4.,  2HV , 50.950, 5.,  2HCR, 52.010, 3.,       P1712  00256
     I 2HMN,54.940,2./                                                  P1712  00257
      DATA ((ATOM(I,J),I=1,3),J=26,51)/                                 P1712  00258
     I 2HFE,55.850,3.,  2HCO,58.940,2.,                                 P1712  00259
     J    2HNI, 58.710, 2.,  2HCU, 63.540, 2.,  2HZN, 65.380, 2.,       P1712  00260
     K    2HGA, 69.720, 3.,  2HGE, 72.600, 4.,  2HAS, 74.920, 3.,       P1712  00261
     L    2HSE, 78.960, 4.,  2HBR, 79.916,-1.,  2HKR, 83.800, 0.,       P1712  00262
     M    2HRB, 85.480, 1.,  2HSR, 87.630, 2.,  2HY , 88.910, 3.,       P1712  00263
     N    2HZR, 91.220, 4.,  2HNB, 92.910, 5.,  2HMO, 95.950, 6.,       P1712  00264
     O    2HTC, 99.000, 7.,  2HRU,101.100, 3.,  2HRH,102.910, 3.,       P1712  00265
     P    2HPD,106.400, 2.,  2HAG,107.880, 1.,  2HCD,112.410, 2.,       P1712  00266
     Q    2HIN,114.820, 3.,  2HSN,118.700, 4.,  2HSB,121.760, 3./       P1712  00267
      DATA ATEM/                                                        P1712  00268
     R    2HTE,127.610, 4.,  2HI ,126.910,-1.,  2HXE,131.300, 0.,       P1712  00269
     S    2HCS,132.910, 1.,  2HBA,137.360, 2.,  2HLA,138.920, 3.,       P1712  00270
     T    2HCE,140.130, 3.,  2HPR,140.910, 3.,  2HND,144.270, 3.,       P1712  00271
     U    2HPM,147.000, 3.,  2HSM,150.350, 3.,  2HEU,152.000, 3.,       P1712  00272
     V    2HGD,157.260, 3.,  2HTB,158.930, 3.,  2HDY,162.510, 3.,       P1712  00273
     W    2HHO,164.940, 3.,  2HER,167.270, 3.,  2HTM,168.940, 3.,       P1712  00274
     X    2HYB,173.040, 3.,  2HLU,174.990, 3.,  2HHF,178.500, 4.,       P1712  00275
     Y    2HTA,180.950, 5.,  2HW ,183.860, 6.,  2HRE,186.220, 7.,       P1712  00276
     Z    2HOS,190.200, 4.,  2HIR,192.200, 4.,  2HPT,195.090, 4.,       P1712  00277
     A    2HAU,197.000, 3.,  2HHG,200.610, 2.,  2HTL,204.390, 1.,       P1712  00278
     B    2HPB,207.210, 2.,  2HBI,209.990, 3.,  2HPO,210.000, 2.,       P1712  00279
     C    2HAT,210.000, 0.,  2HRN,222.000, 0.,  2HFR,223.000, 1.,       P1712  00280
     D    2HRA,226.000, 2.,  2HAC,227.000, 3.,  2HTH,232.000, 4.,       P1712  00281
     E    2HPA,231.000, 5.,  2HU ,238.000, 6.,  2HNP,237.000, 5.,       P1712  00282
     F    2HPU,242.000, 4.,  2HAM,243.000, 3.,  2HCM,247.000, 3.,       P1712  00283
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      G    2HBK,249.000, 3.,   2HCF,251.000, 3.,   2HES,254.000, 0.,    P1712   00284
      H    2HFM,253.000, 0.,   2HMV,256.000, 0./                        P1712   00285
C                                                                       P1712   00286
C      INFORMATION USED IN VARIABLE OUTPUT FORMAT                       P1712   00287
C                                                                       P1712   00288
       DATA FMT/34(1H,4H,3A4,4H,A2,,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1 P1712   00289
     1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF9.,1H ,3HF P1712   00290
     29.,1H ,3HF9.,1H ,3HF9.,1H ,1H)/, F8,F0,F1,F2,F3,F4,F5/1H  ,2H0.,2H P1712   00291
     31,,2H2,,2H3,,2H4,,2H5,/,FMT13/2H13/,FMT9X/3H9X,/,FMTI9/3HI9,/     P1712   00292
       DATA                          FP/4HP, A,4HTM  ,2H  ,1H /         P1712   00293
     1,FT/4HT, C,4HP, D,4HEG K,2H  /,FH/4HH, C,4HAL/G,2H  ,1H /         P1712   00294
     2,FS/4HS, C,4HAL/(,4HG)(K,2H) /,FM/4HM, M,4HOL W,2HT ,1H /         P1712   00295
     3,FV/4H(DLV,4H/DLP,4H)T  ,2H  /,FD/4H(DLV,4H/DLT,2H)P,1H /         P1712   00296
     4,FC/4HCP, ,4HCAL/,4H(G)(,2HK)/,FG/4HGAMM,4HA (S,2H) ,1H /         P1712   00297
     5,FL/4HSON ,4HVEL,,4HM/SE,2HC /                                    P1712   00298
C                                                                       P1712   00299
C      INFORMATION USED IN PERFORMANCE OUTPUT                           P1712   00300
C                                                                       P1712   00301
       DATA FR1/4HPC/P/, FC1/2HCF/,     FN/4HMACH,4H NUM,4HBER ,1H /    P1712   00302
     1,FR/4HCSTA,4HR, F,4HT/SE,2HC  /,FI/4HI, L,4HB-SE,4HC/LB,1H /      P1712   00303
     2,FA/4HIVAC,4H,LB-,4HSEC/,2HLB /,FA1/4HAE/A/,FA2/1HT/              P1712   00304
       END                                                              P1712   00305
```

```
      SUBROUTINE CMBSTN                                                 P1712  00306
C                                                                       P1712  00307
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712  00308
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),..(13),SONVEL(13),TTT(13)  P1712  00309
     2,TCTN(13)                                                         P1712  00310
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  00311
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  00312
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712  00313
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  00314
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  00315
     3 ,ANUM(15,5),PECWT(15),CNTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00316
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  00317
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  00318
     1  KMAT,IMAT,IC1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  00319
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  00320
C                                                                       P1712  00321
C     SET ASSIGNED P                                                    P1712  00322
C                                                                       P1712  00323
      TT = 3800.                                                        P1712  00324
      DO 902 IP = 1,NP                                                  P1712  00325
      PP = P(IP)                                                        P1712  00326
      CALL EQLBRM                                                       P1712  00327
      T(NPT) = TT                                                       P1712  00328
      IF(TT.NE.0.)  GO TO 800                                           P1712  00329
      IF(NPT.EQ.0)  GO TO 1000                                          P1712  00330
  800 K=0                                                               P1712  00331
      IF(IP.EQ.NP.OR.TT.EQ.0.)  GO TO 860                               P1712  00332
      K = NPT                                                           P1712  00333
      IF(NPT.NE.13)  GO TO 870                                          P1712  00334
  860 WRITE (6,6)                                                       P1712  00335
    6 FORMAT (1H1,42X,48HTHEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES P1712  00336
     1   ///)                                                           P1712  00337
      CALL OUT1                                                         P1712  00338
      WRITE (6,863)                                                     P1712  00339
  863 FORMAT (25H0THERMODYNAMIC PROPERTIES//)                           P1712  00340
      CALL OUT2                                                         P1712  00341
      CALL OUT3                                                         P1712  00342
  865 IF(K.EQ.0) GO TO 1000                                             P1712  00343
      NPT = 0                                                           P1712  00344
  870 NPT = NPT + 1                                                     P1712  00345
C                                                                       P1712  00346
C                                                                       P1712  00347
C    SAVE    POSITIONS FOR ESTIMATES OF NEXT POINT                      P1712  00348
      DO     I = 1,NS                                                   P1712  00349
      EN(I,NPT) = EN(I,K)                                               P1712  00350
  880 CONTINUE                                                          P1712  00351
  902 CONTINUE                                                          P1712  00352
 1000 RETURN                                                            P1712  00353
      END                                                               P1712  00354
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      C                                                                   P1712  00355
            SUBROUTINE CPHS                                               P1712  00356
            COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150) P1712  00357
           1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMF(50,2)         P1712  00358
            COMMON/ TSC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),BO(15),BOP(15,2) P1712  00359
           1 ,TM, .OK,TMID,THIGH,PP,CPSUM,OF,EQRA),FPCT,R,RR,HSUBO,AC(2),AM(2) P1712  00360
           2 ,FPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)      P1712  00361
           3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00362
           4 ,RHOP,RMW(15),TLN,JANF                                       P1712  00363
            COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  00364
           1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ P1712  00365
           2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2               P1712  00366
      C                                                                   P1712  00367
            K = 1                                                         P1712  00368
            IF(TT.LE.TMID)K = 2                                           P1712  00369
            KK = 0                                                        P1712  00370
            CPSUM=0.                                                      P1712  00371
         90 IF(COEF(K,1,J).NE.0.)GO TO 97                                 P1712  00372
            IF (IUSE(J).LT.0) GO TO 100                                   P1712  00373
            KK = K                                                        P1712  00374
            K = 1                                                         P1712  00375
            IF (KK.EQ.1) K = 2                                            P1712  00376
         97 CONTINUE                                                      P1712  00377
            IF(JANF.EQ. 0)GO TO 98                                        P1712  00378
            S(J)=COEF(K,1,J)*TLN+COEF(K,7,J)-COEF(K,5,J)/2./TT/TT         P1712  00379
           1+((COEF(K,4,J)/3.0*TT+COEF(K,3,J)/2.0)*TT+COEF(K,2,J))*TT     P1712  00380
            HO(J)=(((COEF(K,4,J)/4.0)*TT+COEF(K,3,J)/3.0)*TT+COEF(K,2,J)/2.0)* P1712  00381
           1TT+COEF(K,1,J)-(COEF(K,5,J)/TT-COEF(K,6,J))/TT                P1712  00382
            CPSUM=CPSUM  ((COEF(K,4,J)*TT+COEF(K,3,J))*TT+COEF(K,2,J))*TT P1712  00383
           1+COEF(K,1,J  -COEF(K,5,J)/TT/TT)*EN(J,NPT)                    P1712  00384
            GO TO 99                                                      P1712  00385
         98 S(J) =  ((((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/2. P1712  00386
           1)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J)          P1712  00387
            HO(J) = ((((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/3. P1712  00388
           1  ) *TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J)  + COEF(K,6,J)/TT    P1712  00389
            CPSUM= CPSUM+((((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF  ,3,J))*TT P1712  00390
           1    + COEF(K,2,J))*TT+ COEF(K,1,J))*EN(J,NPT)                 P1712  00391
         99 CONTINUE                                                      P1712  00392
            IF (KK.EQ.0) GO TO 100                                        P1712  00393
            K = KK                                                        P1712  00394
            KK = 0                                                        P1712  00395
        100 IF(J.EQ.NS) GO TO 200                                         P1712  00396
            J=J+1                                                         P1712  00397
            GO TO 90                                                      P1712  00398
        200 RETURN                                                        P1712  00399
            END                                                           P1712  00400
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      SUBROUTINE DETON                                                P1712  00401
C                                                                     P1712  00402
C                                                                     P1712  00403
C     CHAPMAN-JOUGUET DETONATIONS                                     P1712  00404
C                                                                     P1712  00405
      LOGICAL HP,SP,TP,IDEBUG,NEWR,IONS,MOLES,FROZ,EGL,PSIA,RKT       P1712  00406
      LOGICAL CPCVEQ, CPCVFR, CALCH                                   P1712  00407
C                                                                     P1712  00408
      DIMENSION GM(13),CP(13),H1(13),PUB(13),TUB(13),GM1(13),RRHO(13) P1712  00409
C                                                                     P1712  00410
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)     P1712  00411
     1,GAMMAS(13),P(26),T(26),V(13),PPP(13),HM(13),SONVEL(13),TTT(13) P1712  00412
     2 ,TOTN(13)                                                      P1712  00413
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150) P1712  00414
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)           P1712  00415
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),BO(15),BOP(15,2) P1712  00416
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EGRAT,FPCT,R,RR,HSUBO,AC(2),AM(2) P1712  00417
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)       P1712  00418
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  00419
     4 ,RHOP,RMW(15),TLN,JANF                                         P1712  00420
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  00421
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ   P1712  00422
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                 P1712  00423
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  00424
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                           P1712  00425
      COMMON/CUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FO(4)   P1712  00426
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2      P1712  00427
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FD                     P1712  00428
C                                                                     P1712  00429
      EQUIVALENCE(CP,DATA),(GM,SPIM),(H1,VAC1),(PUB,SUBAR),(TUB,SUPAR) P1712  00430
      EQUIVALENCE(GM1,AEAT),(PCP(14),RRHO)                            P1712  00431
C                                                                     P1712  00432
      DATA FT1/4HT1,D/, FP1/4HP1,A/, FH1/4HH1,C/, FM1/4HH1,M/         P1712  00433
     1 ,  FCP1/4HCP1,/, FG1/4HA1  /, FPP/4HP/P1/, FTT/4HT/T1/         P1712  00434
     2 ,   FUD/4HDET /, FMM/4HM/M1/, FRA/4HRHO//, FRE/4HRHO1/         P1712  00435
     3 ,   FMA/4HMACH/, FMB/4H NO./, IZERO/2H00/                      P1712  00436
C                                                                     P1712  00437
      D(C)= A11*A22-A21*A12                                           P1712  00438
      XX(Y)= (B1*A22-B2*A12)/D(C)                                     P1712  00439
      YY(Z)= (B2*A11-B1*A21)/D(C)                                     P1712  00440
C                                                                     P1712  00441
      NT = 1                                                          P1712  00442
      HSUBO = HSUBO*R                                                 P1712  00443
      CALCH=.TRUE.                                                    P1712  00444
      TT = 0.                                                         P1712  00445
      IF(T(1).EQ.0.)  T(1)=RTEMP(1)                                   P1712  00446
      DO 2 N = 1,NREAC                                                P1712  00447
      IF(NAME(N,5).EQ.IZERO) CALCH = .TRUE.                           P1712  00448
    2 CONTINUE                                                        P1712  00449
      DO 3  IT = 1,26                                                 P1712  00450
      IF (T(IT).EQ.0.) GO TO 7                                        P1712  00451
      NT = IT                                                         P1712  00452
    3 CONTINUE                                                        P1712  00453
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    7 IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GO TO 4                      P1712  00454
      AM1 = AM(2)                                                       P1712  00455
      IF (AM(2).EQ.0.0)AM1 = AM(1)                                      P1712  00456
      GO TO 9                                                           P1712  00457
    4 AM1 = (WP(1)+WP(2))*AM(1)*AM(2)/(WP(2)*AM(1)+WP(1)*AM(2))         P1712  00458
    9 CONTINUE                                                          P1712  00459
      DO 902 IT=1,NT                                                    P1712  00460
      T1= T(IT)                                                         P1712  00461
      TT = T1                                                           P1712  00462
      IF (CALCH) CALL HCALC                                             P1712  00463
      CP1 = (WP(1)*AC(1)+WP(2)*AC(2))/(WP(1)+WP(2))                     P1712  00464
      DO 902 IP=1,NP                                                    P1712  00465
      P1= P(IP)                                                         P1712  00466
      H1(NPT) = HSUB0                                                   P1712  00467
      TUB(NPT)=T1                                                       P1712  00468
      PUB(NPT)=P1                                                       P1712  00469
      CP(NPT) = CP1*R                                                   P1712  00470
      ITR= 0                                                            P1712  00471
      TT= 3800.                                                         P1712  00472
      PP1= 15.                                                          P1712  00473
      PP= PP1*P1                                                        P1712  00474
      HSUB0 = H1(NPT)/R + .75*T1*PP1/AM1                                P1712  00475
      TP = .FALSE.                                                      P1712  00476
      HP= .TRUE.                                                        P1712  00477
      CALL EQLBRM                                                       P1712  00478
      HSUB0 = H1(NPT)                                                   P1712  00479
      HP= .FALSE.                                                       P1712  00480
      IF(TT.EQ.0.) GO TO 1000                                           P1712  00481
      GAM= GAMMAS(NPT)                                                  P1712  00482
      TT1= TT/T1                                                        P1712  00483
      II= 0                                                             P1712  00484
      TEM=TT1-.75*PP1/(CPR(NPT)*AM1)                                    P1712  00485
      AMM=WM(NPT)/AM1                                                   P1712  00486
      IF(IDEBUG) WRITE(6,190)                                           P1712  00487
  190 FORMAT(33H1DETONATION VELOCITY CALCULATIONS /11X,4HP/P1,17X,4HT/T1 P1712  00488
     1)                                                                 P1712  00489
      IF(IDEBUG) WRITE(6,203) II,PP1,TT1                                P1712  00490
C                                                                       P1712  00491
  200 DO 202 II=1,4                                                     P1712  00492
      ALFA=AMM/TT1                                                      P1712  00493
      PP1= (1.+GAM)*(1.+(1.-4.*GAM*ALFA/(1.+GAM)**2)**.5)/(2.*GAM*ALFA)  P1712  00494
      RK=PP1*ALFA                                                       P1712  00495
      TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)                  P1712  00496
      IF(IDEBUG) WRITE(6,203) II,PP1,TT1                                P1712  00497
  203 FORMAT (I5,2E20.8)                                                P1712  00498
  202 CONTINUE                                                          P1712  00499
      TP= .TRUE.                                                        P1712  00500
      TT= T1*TT1                                                        P1712  00501
      RR1 = PP1*AMM/TT1                                                 P1712  00502
C                                                                       P1712  00503
  205 ITR= ITR+1                                                        P1712  00504
      PP= P1*PP1                                                        P1712  00505
      CALL EQLBRM                                                       P1712  00506
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```
      IF (NPT.EQ.0) GO TO 1000
      IF (TT.EQ.0.) GO TO 860
      GAM= GAMMAS(NPT)
C     IF(CPCVFR)GAM= CPRF(NPT)/(CPRF(NPT)-1./WM(NPT))
C     IF(CPCVEQ)GAM= -GAMMAS(NPT)*DLVPT(NPT)
      AMM= WM(NPT)/AM1
      RR1= PP1*AMM/TT1
      A11= 1./PP1 + GAM*RR1*DLVPT(NPT)
      A12= GAM*RR1*DLVTP(NPT)
      A21= .5*GAM*(RR1**2-1.-DLVPT(NPT)*(1.+RR1**2))+DLVTP(NPT)-1.
      A22=-.5*GAM*DLVTP(NPT)*(RR1**2+1.)-WM(NPT)*CPR(NPT)
      B1= 1./PP1-1.+GAM*(RR1-1.)
      B2= WM(NPT)*(HSUM(NPT)-H1(NPT)/R)/TT-.5*GAM*(RR1*RR1-1.)
      X1 = XX(Y)
      X2 = YY(Z)
      ALAM= 1.
      TEM = X1
      IF(TEM.LT.0.)  TEM = -TEM
      IF(X2.GT.TEM)  TEM=X2
      IF (-X2.GT.TEM) TEM = -X2
      IF(TEM.GT.0.4) ALAM=.4/TEM
      PP1= PP1*EXP(X1*ALAM)
      TT1= TT1*EXP(X2*ALAM)
      TT = T1*TT1
      US = (RR*GAM*T1/WM(NPT))**.5
      UD= RR1*US
      IF(IDEBUG) WRITE(6,10) ITR
   10 FORMAT (21H0   ITERATION NUMBER=I2        )
      IF(IDEBUG) WRITE(6,30) PP1,TT1,RR1,X1,X2,US
   30 FORMAT(6X,4HP/P1,10X,1H= E20.8/6X,4HT/T1,10X,1H= E20.8/6X,8HRHO/RH
     101,6X,1H= E20.8/6X,11HDEL LN P/P1,3X,1H=E20.8/6X,11HDEL LN T/T1,3X
     2,1H=E20.8/6X,2HUS,12X,1H=E20.8)
C
C     CONVERGENCE TEST
C
      IF(ITR.LE.10 .AND. TEM.GT.0.5E-04)  GO TO 205
      RRHO(NPT)=RR1
      IF (CP(NPT).EQ.0.) GO TO 40
      GM1(NPT) = CP(NPT) /(CP(NPT)-R/AM1)
      VMCC(NPT) = UD/(RR*GM1(NPT)*T1/AM1)**.5
      GO TO 41
   40 GM1(NPT) = 0.
      VMCC(NPT) = 0.
      GO TO 150
C
C   DERIVATIVES
C
   41 IF(IDEBUG) WRITE(6,55)
   55 FORMAT (17H0   DERIVATIVE OF,15X,4HLN P,16X,4HLN T,16X,2HUD,
    1         /9X,2HBY )
      B1= 1./PP1-GAM*RR1
      B2= GAM*RR1**2
      X1 = XX(Y)
```

```
      X2 = YY(Z)
      AA= .5*(1.-DLVPT(NPT))
      BB= -.5*DLVTP(NPT)
      DUC= UD*(AA*X1+BB*X2-1.)
      X1= X1-1.0
      IF(IDEBUG) WRITE(6,81) X1,X2,DUD
   81 FORMAT(6X,13HLNP1 AT T1,H1,6X,1H=,3E17.8)
      B1= GAM*RR1
      B2= -B1*RR1-WM(NPT)*CP(NPT)/(R*TT1)
      X1 = XX(Y)
      X2 = YY(Z)
      DUD= UD*(AA*X1+BB*X2+1.)
      X2= X2-1.
      IF(IDEBUG) WRITE(6,84) X1,X2,DUD
   84 FORMAT(6X,16HLNT1 AT P1,H1,M1,3X,1H=3E17.8)
      B1= 0.
      B2= -WM(NPT)/(R*TT)
      X1 = XX(Y)*1000.
      X2 = YY(Z)*1000.
      DUD= UD*(AA*X1+BB*X2)
      IF(IDEBUG) WRITE(6,85) X1,X2,DUD
   85 FORMAT (6X,20HH1    AT T1,P1,H1    =3E17.8)
C
  150 K = 0
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860
      K = NPT
      IF(NPT.NE.13)  GO TO 870
C
C  OUTPUT
C
  860 WRITE (6,5)
    5 FORMAT(1H1,42X,46HDETONATION PROPERTIES OF AN IDEAL REACTING GAS )
      CALL OUT1
      WRITE(6,46)
   46 FORMAT(13H UNBURNED GAS//)
      FMT(4)=FMT13
      FMT(5)=F8
      FMT(7)=F4
      WRITE(6,FMT)FP1,FP(2),F8,F8,(PUB(J),J=1,NPT)
      FMT(7)=F2
      WRITE(6,FMT)FT1,FT(2),F8,F3,(TUB(J),J=1,NPT)
      WRITE(6,FMT)FH1,FH(2),F8,F8,(H1(J), J=1,NPT)
      DO 56 I=1,NPT
      V(I)=AM1
      SONVEL(I)=    (RR*GM1(I)*TUB(I)/AM1)**.5
   56 CONTINUE
      FMT(7)=F3
      WRITE(6,FMT) FM1,FM(2),FM(3),F8,(V(J),J=1,NPT)
      FMT(7)=F4
      WRITE(6,FMT)FCP1,FC(2),FC(3),FC(4),(CP(J),J=1,NPT)
      WRITE(6,FMT)FG(1),FG1,F8,F8,(GM1(J),J=1,NPT)
      FMT(7)=F1
      WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT)
```

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      WRITE(6,58)                                                        P1712  00613
   58 FORMAT(11H0BURNED GAS//)                                          P1712  00614
      FMT(4)=FMT(6)                                                      P1712  00615
      CALL OUT2                                                          P1712  00616
      WRITE(6,68)                                                        P1712  00617
   68 FORMAT(22H0DETONATION PARAMETERS //)                              P1712  00618
      FMT(7)=F3                                                          P1712  00619
      DO 70 I=1,NPT                                                      P1712  00620
      V(I)= PPP(I)/PUB(I)                                                P1712  00621
      PCP(I)=TTT(I)/TUB(I)                                               P1712  00622
      SONVEL(I)=SONVEL(I)*RRHO(I)                                        P1712  00623
   70 CONTINUE                                                           P1712  00624
      WRITE(6,FMT)FPP,FB,FB,FB,(V(J),J=1,NPT)                            P1712  00625
      WRITE(6,FMT)FTT,FB,FB,FB,(PCP(J),J=1,NPT)                          P1712  00626
      DO 73 I=1,NPT                                                      P1712  00627
      V(I)=WM(I)/AM1                                                     P1712  00628
   73 CONTINUE                                                           P1712  00629
      FMT(7)=F4                                                          P1712  00630
      WRITE(6,FMT)FMM,FB,FB,FB,(V(J),J=1,NPT)                            P1712  00631
      WRITE(6,FMT)FRA,FR3,FB,FB,(RRHO(J),J=1,NPT)                        P1712  00632
      WRITE(6,FMT)FMA,FMB,FB,FB,(VMOC(J),J=1,NPT)                        P1712  00633
      FMT(7)=F1                                                          P1712  00634
      WRITE(6,FMT) FUD,FL(2),FL(3),FL(4),(SONVEL(J),J=1,NPT)             P1712  00635
      EQL=.TRUE.                                                         P1712  00636
      CALL OUT3                                                          P1712  00637
  865 IF(K.EQ.0) GO TO 1000                                              P1712  00638
      WRITE(6,868)                                                       P1712  00639
  868 FORMAT(1H1)                                                        P1712  00640
      NPT = 0                                                            P1712  00641
  870 NPT = NPT + 1                                                      P1712  00642
C                                                                        P1712  00643
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT                        P1712  00644
C                                                                        P1712  00645
      DO 880 I = 1,NS                                                    P1712  00646
      EN(I,NPT) = EN(I,K)                                                P1712  00647
  880 CONTINUE                                                           P1712  00648
  902 CONTINUE                                                           P1712  00649
 1000 TP = .FALSE.                                                       P1712  00650
      RETURN                                                             P1712  00651
      END                                                                P1712  00652
```

```
      C                                                               P1712   00653
        SUBROUTINE EQLBRM                                             P1712   00654
      C ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES    P1712   00655
      C                                                               P1712   00656
      C  DOUBLE PRECISION X,G                                         P1712   00657
        LOGICAL HP,SP,TP,IDEBUG,CONVG,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP P1712   00658
        LOGICAL ISING,IC                                              P1712   00659
      C                                                               P1712   00660
        DIMENSION PROW(18)                                            P1712   00661
      C                                                               P1712   00662
        COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)   P1712   00663
       1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712   00664
       2,TOTN(13)                                                     P1712   00665
        COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150 ,H0(150) P1712   00666
       1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)         P1712   00667
        COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) P1712   00668
       1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712   00669
       2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)     P1712   00670
       3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712   00671
       4 ,RHOP,RMW(15),TLN,JANF                                       P1712   00672
        COMMON /DOUBLE/ G(20,21), X(20)                               P1712   00673
        COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712   00674
       1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ P1712   00675
       2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2               P1712   00676
        COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712   00677
       1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0                         P1712   00678
      C                                                               P1712   00679
        DATA ITER/4HITER/,IE/1HE/,SMALNO/1.E-6/,SMNOL/-13.815511/     P1712   00680
      C                                                               P1712   00681
        SIZE= 18.5                                                    P1712   00682
        ISING = .FALSE.                                               P1712   00683
        ENNL = ALOG(ENN)                                              P1712   00684
        LOGV = .FALSE.                                                P1712   00685
        PP.N = ALOG(PP)                                               P1712   00686
        TLN = ALOG(TT)                                                P1712   00687
        CONVG = .FALSE.                                               P1712   00688
        ITNUMB = ITN                                                  P1712   00689
        IF(IC)  GO TO 966                                             P1712   00690
        IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33                      P1712   00691
        L = L+1                                                       P1712   00692
        IQ1 = IQ1+1                                                   P1712   00693
        DO 499 J = 1,NS                                               P1712   00694
        IF (A(L,J) .EQ.0.) GO TO 499                                  P1712   00695
        EN(J,NPT) = SMALNO                                            P1712   00696
        ENLN(J) = SMNOL                                               P1712   00697
        IUSE(J) = 0                                                   P1712   00698
   499  CONTINUE                                                      P1712   00699
    33  IF(NPT.EQ.1 .AND. IDEBUG) WRITE(6,244) (LLMT(I),I=1,L),ITER   P1712   00700
   244  FORMAT (4HOPT ,14(5X,A4))                                     P1712   00701
    43  TM = ALOG(PP/ENN)                                             P1712   00702
        J = 1                                                         P1712   00703
        IF(.NOT.TP) CALL CPHS                                         P1712   00704
        IF(TP.AND.(CONVG.OR.ITNUMB.EQ.ITN)) CALL CPHS                 P1712   00705
```

```
      IF(IC)  GO TO 171                                          P1712  00706
      IF (.NOT.CONVG.OR.JSOL.EQ.0) GO TO 62                      P1712  00707
      ENSOL = EN(JSOL,NPT)                                       P1712  00708
      EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)                   P1712  00709
      IUSE(JLIQ) = -IUSE(JLIQ)                                   P1712  00710
      IQ1 = IQ1-1                                                P1712  00711
      DLVTP(NPT) = 0.                                            P1712  00712
      CPR(NPT) = 0.                                              P1712  00713
      GAMMAS(NPT) = 0.                                           P1712  00714
      LOGV = .TRUE.                                              P1712  00715
   62 CALL MATRIX                                                P1712  00716
      NUMB = ITN-ITNUMB+1                                        P1712  00717
      IF(.NOT.CONVG)    GO TO 67                                 P1712  00718
      IF (LOGV.AND.JSOL.EQ.0) GO TO 63                           P1712  00719
      DO 182  I=1,L                                              P1712  00720
      PROW(I) = G(IQ1,I)                                         P1712  00721
  182 CONTINUE                                                   P1712  00722
      IF (.NOT.LOGV) GO TO 67                                    P1712  00723
C                                                                P1712  00724
C     LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT           P1712  00725
C                                                                P1712  00726
   63 G(IQ1,IQ2) = ENN                                           P1712  00727
      IQ = IQ1 - 1                                               P1712  00728
      DO 777 I = 1,IQ                                            P1712  00729
      G(I,IQ2) = G(I,IQ1)                                        P1712  00730
  777 CONTINUE                                                   P1712  00731
   67 IF (.NOT.IDEBUG) GO TO 72                                  P1712  00732
      WRITE(6,772) NUMB                                          P1712  00733
  772 FORMAT (11H0ITERATION  ,I3,6X,7HMATRIX //)                 P1712  00734
      DO 911  I=1,IMAT                                           P1712  00735
  911 WRITE (6,73)  (G(I,K),K=1,KMAT)                            P1712  00736
   72 IF(CONVG)  IMAT=IMAT-1                                     P1712  00737
      ITST = IMAT                                                P1712  00738
      CALL MGAUSD                                                P1712  00739
      IF(ITST.NE.IMAT)  GO TO 774                                P1712  00740
      IF(.NOT.IDEBUG.OR.CONVG)  GO TO 773                        P1712  00741
      WRITE (6,373) (LLMT(I),I=1,L)                              P1712  00742
  373 FORMAT (7H0PI    ,9(A4,10X))                               P1712  00743
      WRITE (6,73) (X(I),I=1,IMAT)                               P1712  00744
   73 FORMAT (9E14.6)                                            P1712  00745
  773 IF(.NOT.CONVG)  GO TO 85                                   P1712  00746
      IF(LOGV)  GO TO 171                                        P1712  00747
  174 SUM = 0.                                                   P1712  00748
      DO 175 J=1,L                                               P1712  00749
      SUM = SUM+PROW(J)*X(J)                                     P1712  00750
  175 CONTINUE                                                   P1712  00751
      DLVTP(NPT) = 1.+G(IQ2,IQ1)/ENN-SUM/ENN  - X(IQ1)           P1712  00752
      CPR(NPT) = G(IQ2,IQ2)                                      P1712  00753
      DO 176 J=1,IQ1                                             P1712  00754
      CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)                          P1712  00755
  176 CONTINUE                                                   P1712  00756
      LOGV = .TRUE.                                              P1712  00757
      GO TO 62                                                   P1712  00758
```

```
C                                                                    P1712  00759
C   SINGULAR MATRIX                                                  P1712  00760
C                                                                    P1712  00761
  774 IF(.NOT.CONVG)  GO TO 775                                      P1712  00762
      WRITE(6,172)                                                   P1712  00763
  172 FORMAT(25H0DERIVATIVE MATRIX SINGULAR )                        P1712  00764
      IC = .TRUE.                                                    P1712  00765
      GO TO 171                                                      P1712  00766
  775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 371   P1712  00767
      WRITE(6,874)                                                   P1712  00768
  874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE P1712  00769
     1BEEN INCLUDED ON AN INSERT CARD, RESTART )                     P1712  00770
      GO TO 873                                                      P1712  00771
  871 WRITE (6,74)                                                   P1712  00772
   74 FORMAT(16H0SINGULAR MATRIX)                                    P1712  00773
      IF(IC)  GO TO 873                                              P1712  00774
      IF (ISING) GO TO 997                                           P1712  00775
      NTZERO = 0                                                     P1712  00776
  965 DO 970 JJ = 1, NS                                              P1712  00777
      IF(IUSE(JJ)) 970,968,967                                       P1712  00778
  967 IF(EN(JJ,NPT).EQ.0.)  GO TO 873                                P1712  00779
      GO TO 969                                                      P1712  00780
  968 IF(EN(JJ,NPT).NE.0.)  GO TO 969                                P1712  00781
      EN(JJ,NPT) = SMALNO                                            P1712  00782
      ENLN(JJ) = SMNOL                                               P1712  00783
      GO TO 970                                                      P1712  00784
  969 NTZERO = NTZERO+1                                              P1712  00785
  970 CONTINUE                                                       P1712  00786
      IF(.NOT.IC)  GO TO 971                                         P1712  00787
      IC = .FALSE.                                                   P1712  00788
      GO TO 43                                                       P1712  00789
  971 ISING = .TRUE.                                                 P1712  00790
      WRITE (6,776)                                                  P1712  00791
  776 FORMAT (8H0RESTART)                                            P1712  00792
      GO TO 43                                                       P1712  00793
  997 IF(NTZERO.NE.(L-1))  GO TO 873                                 P1712  00794
      IF(EQRAT.GT.1.00001.OR.EQRAT.LT.0.99999) GO TO 873             P1712  00795
      ENN=0.                                                         P1712  00796
      NEN = 0                                                        P1712  00797
      DO 83  I=1,L                                                   P1712  00798
      JEN=0                                                          P1712  00799
      DO 80  J=1,NS                                                  P1712  00800
      IF(EN(J,NPT).EQ.0.)  GO TO 80                                  P1712  00801
      IF(A(I,J).EQ.0.)  GO TO 83                                     P1712  00802
      IF(JEN.NE.0)  GO TO 83                                         P1712  00803
      JEN = J                                                        P1712  00804
   80 CONTINUE                                                       P1712  00805
      NEN = NEN+1                                                    P1712  00806
      EN(JEN,NPT) = B0(I)/A(I,JEN)                                   P1712  00807
   83 CONTINUE                                                       P1712  00808
      IF(NEN.LT.NTZERO)  GO TO 373                                   P1712  00809
      CONVG = .TRUE.                                                 P1712  00810
      IC = .TRUE.                                                    P1712  00811
```

```
      HSUM(NPT) = 0.
      DO 84  J=1,NS
      IF(EN(J,NPT).EQ.0.)  GO TO 84
      ENN = EN(J,NPT)+ENN
      TEM = EN(J,NPT)
      ENLN(J) = ALOG(TEM)
      HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*H0(J)
   84 CONTINUE
      TM = ALOG(PP/ENN)
      GO TO 43
   85 ITNUMB= ITNUMB-1
C
C     OBTAIN CORRECTIONS TO THE ESTIMATES
C
      KK = L + 1
      DLNT= X(IQ2)
      IF (TP) DLNT=0.
      DO 101 J=1,NS
      IF (IUSE(J)) 101,98,100
   98 DELN(J) = H0(J)*DLNT-H0(J)+S(J)-ENLN(J)-TM+X(IQ1)
      DO 99 K=1,L
      DELN(J)= DELN(J)+A(K,J)*X(K)
   99 CONTINUE
      GO TO 101
  100 DELN(J) = X(KK)
      KK = KK + 1
  101 CONTINUE
      AMBDA= 1.
      AMBDA1= 1.
      SUM = X(IQ1)
      IF(SUM.LT.0.)  SUM=-SUM
      IF(DLNT.GT.SUM)  SUM=DLNT
      IF(-DLNT.GT.SUM)  SUM=-DLNT
      DO 917 J=1,NS
      IF (IUSE(J).NE.0) GO TO 917
      IF((EN(J,NPT).GT.0.).AND.DELN(J).GT.SUM)  SUM = DELN(J)
      IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GO TO 917
      SUM1 = (-9.212-ENLN(J)+ENNL)/(DELN(J)-X(IQ1))
      IF(SUM1.LT.0.)  SUM1=-SUM1
      IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1
  917 CONTINUE
      IF(SUM.GT.2.)AMBDA=2./SUM
      IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1
      IF (.NOT.IDEBUG) GO TO 111
      WRITE(6,923) TT,ENN,ENNL,PP,PPLN,AMBDA
  923 FORMAT (3H0T=,E15.8,6H  ENN=,E15.8,7H  ENNL=E15.8,5H  PP=,E15.8,
     1 7H  PPLN=E15.8,8H  AMBDA=E15.8 )
      WRITE (6,924)
  924 FORMAT(1H0,18X,2HNI,12X,5HLN NI,8X,9HDEL LN NI,10X,4HH/RT,9X,4HS0/
     1R,12X,6H-G0/RT,9X,5H-G/RT  )
      DO 926 J=1,NS
      FNEG1 = S(J)-H0(J)
      FNEG2 = FNEG1
```

```
      IF(IUSE(J).EQ.0)  FNEG2=FNEG2-ENLN(J)-TM
      WRITE (6,925) SUB(J,1),SUB(J,2),
     1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),H0(J),S(J),FNEG1,FNEG2
  925 FORMAT (1X,3A4,7E15.6)
  926 CONTINUE
      WRITE (6,110)
  110 FORMAT(1H0)
C
C     APPLY CORRECTIONS TO ESTIMATES
C
  111 SUM = 0.
      DO 113 J=1,NS
      IF (IUSE(J)) 113,112,114
  112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)
      EN(J,NPT) = 0.
      IF((ENLN(J)-ENNL+SIZE).LE.0.)  GO TO 113
      EN(J,NPT) = EXP(ENLN(J))
      SUM = SUM+EN(J,NPT)
      GO TO 113
  114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)
  113 CONTINUE
      SUMN = SUM
      IF (TP) GO TO 115
      TLN= TLN+AMBDA*DLNT
      TT     = EXP(TLN)
  115 ENNL = ENNL+AMBDA*X(IG1)
      ENN = EXP(ENNL)
      IF (LLMT(L).NE.IE) GO TO 116
C
C     CHECK ON REMOVING IONS
C
      DO 1116 J = 1,NS
      IF (A(L,J).EQ.0.) GO TO 1116
      IF (EN(J,NPT).GT.0.) GO TO 116
 1116 CONTINUE
      DO 1118  J=1,NS
      IF(A(L,J).NE.0.) IUSE(J) = -10000
 1118 CONTINUE
      L = L-1
      IG1 = IG1-1
      GC TO 43
C
C     TEST FOR CONVERGENCE
C
  116 IF (ITNUMB.EQ.0) GO TO 13
      IF (AMBDA.LT.1.) GO TO 43
      SUM = (ENN-SUMN)/ENN
      IF (SUM.LT.0.) SUM = -SUM
      IF (SUM.GT.0.5E-5) GO TO 43
      DO 130 J=1,NS
      IF (IUSE(J).LT.0) GO TO 130
      AA= DELN(J)/SUMN
      IF(AA.LT.0.)  AA=-AA
```

```
      IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)
  129 IF(AA.GT.0.5E-5)  GO TO 43
  130 CONTINUE
   13 CONVG= .TRUE.
      IF(TT.LT.TLOW.OR.TT.GT.THIGH.AND.IDEBUG) WRITE(6,306) TT,NPT
  306 FORMAT(17H0THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)
      IF(ITNUM3.NE.3) GO TO 165
      WRITE(6,973) ITN,NPT
  973 FORMAT(1HL,I2,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREME
     1NTS FOR THE POINT        I5)
      IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.)  GO TO 873
      WRITE(6,874)
      TT = T(1)
      RETURN
C
C     CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
C
  160 IF(NC.EQ.0) GO TO 143
      SIZEF = 0.
      INC = 0
      DO 170 J = 1,NS
      IF (IUSE(J).EQ.0 .OR. IUSE(J).EQ.-10000) GO TO 170
      INC = INC + 1
      IF(IDEBUG) WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),
     1IUSE(J),EN(J,NPT)
  144 FORMAT (1H0,3A4,2F10.3,3X,6HIUSE=,I4,E15.7)
      IF (EN(J,NPT))  146,148,159
  146 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147
      JSOL = 0
      JLIQ = 0
  147 ICI = ICI - 1
      EN(J,NPT) = 0.
      GO TO 166
  148 KG = 1
      IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154
  151 IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153
      KG = -1
  154 JKG = J + KG
      IF (EN(JKG,NPT).LT.0.) GO TO 170
      TMELT = TEMP(INC,1)
      IMP = INC + KG
      IF(TMELT.EQ.TEMP(IMP,2  )) GO TO 158
      TMELT = TEMP(INC,2)
      IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157
      WRITE (6,156)
  156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER  )
C
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 (HP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP)  GO TO 1165
      IF (TT.LE.TMELT-150.) GO TO 1165
```

```
            JSOL = J                                                   P1712  00971
            JLIQ = JKG                                                 P1712  00972
            GO TO 159                                                  P1712  00973
C                                                                      P1712  00974
C    JTH SPECIES A LIQUID(EN=0), (J+KG)TH SPECIES A SOLID (EN IS +)    P1712  00975
C                                                                      P1712  00976
      158 IF (TT.LT.TMELT) GO TO 169                                   P1712  00977
          IF (TP.AND.TT.EQ.TMELT) GO TO 169                            P1712  00978
          IF (TP)  GO TO 1165                                          P1712  00979
          IF (TT.GE.TMELT+150.) GO TO 1165                             P1712  00980
          JSOL = JKG                                                   P1712  00981
          JLIQ = J                                                     P1712  00982
      159 TLN = ALOG (TMELT)                                           P1712  00983
          TT = TMELT                                                   P1712  00984
          EN(JKG,NPT) = .5 * EN(JKG,NPT)                               P1712  00985
          EN(J,NPT) = EN(JKG,NPT)                                      P1712  00986
          GO TO 165                                                    P1712  00987
C                                                                      P1712  00988
C    WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN                    P1712  00989
C                                                                      P1712  00990
     1165 EN(J,NPT) = EN (JKG, NPT)                                    P1712  00991
          IUSE(J) = -IUSE(J)                                           P1712  00992
          IUSE (JKG) = -IUSE(JKG)                                      P1712  00993
          EN(JKG,NPT)= 0.                                              P1712  00994
          GO TO 40                                                     P1712  00995
      153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169    P1712  00996
          IF (TT.GT.TEMP(INC,2)) GO TO 169                             P1712  00997
C                                                                      P1712  00998
C                                                                      P1712  00999
          SUM = 0.                                                     P1712  01000
          DO 167 I = 1,L                                               P1712  01001
          SUM = SUM + A(I,J)*X(I)                                      P1712  01002
      167 CONTINUE                                                     P1712  01003
          DELF = H0(J)-S(J)-SUM                                        P1712  01004
          IF(IDEBUG) WRITE(6,168)DELF,SIZEF                            P1712  01005
      168 FORMAT (17H G0-SUM(AIJ*PI) =E15.7,10X,18HPREVIOUS DELTA G =,E15.7) P1712  01006
          IF(DELF.GE.SIZEF .OR. DELF.GE.0.) GO TO 169                  P1712  01007
          SIZEF = DELF                                                 P1712  01008
          JDELF = J                                                    P1712  01009
      169 IF(INC.EQ.NC) GO TO 1160                                     P1712  01010
      170 CONTINUE                                                     P1712  01011
     1160 IF (SIZEF.EQ.0.) GO TO 143                                   P1712  01012
          J = JDELF                                                    P1712  01013
      165 IC1 = IC1 + 1                                                P1712  01014
      166 IUSE(J) = - IUSE(J)                                          P1712  01015
       40 CONVG = .FALSE.                                              P1712  01016
      143 TN = NUMB                                                    P1712  01017
          IF(IDEBUG) WRITE(6,771) NPT, (X(IL),IL=1,L), TN              P1712  01018
      771 FORMAT (I3,14F9.3)                                           P1712  01019
          ITNUMB = ITN                                                 P1712  01020
          GO TO 43                                                     P1712  01021
C                                                                      P1712  01022
C         CALCULATE EQUILIBRIUM PROPERTIES                             P1712  01023
```

57

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      C                                                                P1712  01024
  171 SSUM(NPT) = 0.                                                   P1712  01025
      IF(JLIQ.NE.0) EN(JSOL,NPT)=ENSOL                                 P1712  01026
      DO 183 J=1,NS                                                    P1712  01027
      IF (NPT.EQ.1) SS0 = SS0 + EN(J,1)*S(J)                           P1712  01028
      SS = S(J)                                                        P1712  01029
      IF(IUSE(J).EQ.0)  SS=SS-ENLN(J)-T4                               P1712  01030
      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)                               P1712  01031
  183 CONTINUE                                                         P1712  01032
      IF(.NOT.IC)  GO TO 178                                           P1712  01033
      DLVPT(NPT) = -1.                                                 P1712  01034
      DLVTP(NPT) = 1.                                                  P1712  01035
      CPR(NPT) = CPSUM                                                 P1712  01036
      GO TO 199                                                        P1712  01037
  178 SUM = 0.                                                         P1712  01038
      DO 179 J = 1,L                                                   P1712  01039
      SUM = SUM + PROD(J)*X(J)                                         P1712  01040
  179 CONTINUE                                                         P1712  01041
      DLVPT(NPT) = -2.+SUM/ENN+ X(IQ1)                                 P1712  01042
  184 IF(JLIQ.EQ.0)  GO TO 199                                         P1712  01043
      IUSE(JLIQ) = -IUSE(JLIQ)                                         P1712  01044
      HSUM(NPT) = HSUM(NPT)+EN(JLIQ,NPT)*(H0(JLIQ)-H0(JSOL))           P1712  01045
      IQ1 = IQ1+1                                                      P1712  01046
      GAMMAS(NPT) = -1./DLVPT(NPT)                                     P1712  01047
      GO TO 186                                                        P1712  01048
  199 GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))      P1712  01049
  186 TTT(NPT) = TT                                                    P1712  01050
      PPP(NPT) = PP                                                    P1712  01051
      CPRF(NPT) = CPSUM                                                P1712  01052
      HSUM(NPT) = HSUM(NPT)*TT                                         P1712  01053
      WM(NPT) = 1./ENN                                                 P1712  01054
  200 IF (.NOT.IDEBUG) RETURN                                          P1712  01055
      WRITE(6,201) NPT,PCP(NPT),PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NP P1712  01056
     1T),DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT)                             P1712  01057
  201 FORMAT (7H0POINT=I3,3X,4HPCP=E13.6,3X,2HP=E13.6,3X,2HT=E13.6,3X,4H P1712  01058
     1H/R=E13.6,3X,4HS/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT P1712  01059
     2=E13.6,3X,6HDLVTP=E13.6,3X,9HGAMMA(S)=E13.6 )                    P1712  01060
      GO TO 1000                                                       P1712  01061
      C                                                                P1712  01062
      C      ERROR, SET TT=0                                           P1712  01063
      C                                                                P1712  01064
  873 TT=0.                                                            P1712  01065
      NPT = NPT-1                                                      P1712  01066
 1000 RETURN                                                           P1712  01067
      END                                                              P1712  01068
```

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      SUBROUTINE FROZEN                                                      P1712  01069
C                                                                            P1712  01070
C                                                                            P1712  01071
C     (FROZEN COMPOSITION EXPANSION ONLY)                                    P1712  01072
C                                                                            P1712  01073
      LOGICAL EQL,FROZ,CONVG                                                 P1712  01074
C                                                                            P1712  01075
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)            P1712  01076
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)       P1712  01077
     2,TCTN(13)                                                              P1712  01078
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HO(150)        P1712  01079
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)                  P1712  01080
      COMMON/MISC/ENN,SUMN,TT,SN,ATOM(3,101),ELMT(15),BO(15),BOP(15,2)       P1712  01081
     1 ,TM,TLOW,TMID,THIGH,PC,C SUM,OF,EQRAT,FPCT,R,RR,HSUBO,AC(2),AM(2)     P1712  01082
     2 ,HPP(2),RHO(2),VMIN(2),  LS(2),WP(2),DATA(22),NAME(15,5)              P1712  01083
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)     P1712  01084
     4 ,RHOP,RMW(15),TLN,JANF                                                P1712  01085
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,     P1712  01086
     1  KMAT,IMAT,IQI,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ          P1712  01087
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                        P1712  01088
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)     P1712  01089
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                                  P1712  01090
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)          P1712  01091
     1   ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2            P1712  01092
     2   ,FRI,FCI,FN(4),FR(4),FA(4),FI(4),FMT9X,FO                           P1712  01093
      ITROT = 3                                                              P1712  01094
      EQL =.FALSE.                                                           P1712  01095
      NPT = 2                                                                P1712  01096
       TT = TTT(1)                                                           P1712  01097
      TLN=ALOG(TT)                                                           P1712  01098
      GAMMAS(1) = CPRF(1)/(CPRF(1)-1./WM(1))                                 P1712  01099
      CPR(1) = CPRF(1)                                                       P1712  01100
      PCP(2) = ((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))               P1712  01101
      DATA(1) = 2./(GAMMAS(1) + 1.)                                          P1712  01102
      TLN = TLN + ALOG(DATA(1))                                              P1712  01103
      DO 902  IP=2,NP                                                        P1712  01104
      IF(NPT.EQ.2)  GO TO 45                                                 P1712  01105
      PCP(NPT) = P(1)/P(IP)                                                  P1712  01106
   45 CONVG = .FALSE.                                                        P1712  01107
      PCPLN= ALOG(PCP(NPT))                                                  P1712  01108
      SO = SSO -PCPLN/WM(1)                                                  P1712  01109
      SUMH = 0.                                                              P1712  01110
   51 TT=EXP(TLN)                                                            P1712  01111
      SUMS=0.                                                                P1712  01112
      J = 1                                                                  P1712  01113
      NNN = NPT                                                              P1712  01114
      NPT = 1                                                                P1712  01115
      CALL CPHS                                                              P1712  01116
      NPT = NNN                                                              P1712  01117
      DO 60 J=1,NS                                                           P1712  01118
      IF(EN(J,1).EQ.0.)  GO TO 60                                            P1712  01119
      SUMS = SUMS + S(J)*EN(J,1)                                             P1712  01120
      IF(CONVG) SUMH=SUMH+HO(J)*EN(J,1)                                      P1712  01121
```

```
   60 CONTINUE
      IF (CONVG) GO TO 81
      DLNT=(SUMS-S0)/CPSUM
      TLN=TLN-DLNT
      IF(DLNT.LT.0.) DLNT=-DLNT
      IF(DLNT.LT.0.5E-4)  CONVG=.TRUE.
      GO TO 51
   81 TTT(NPT)= TT
      SSUM(NPT)= SSUM(1)
      HSUM(NPT)= TT*SUMH
      GAMMAS(NPT)= CPSUM/(CPSUM-1./WM(1))
      IF(IP.GT.2)  GO TO 90
C
C     THROAT CALCULATIONS
C
      DH = HSUM(1)-HSUM(2)
      DHSTAR = DH-(GAMMAS(2)*TT/(2.*WM(1)))
      DH = DHSTAR/DH
      IF(DH.LT.0.)  DH=-DH
      IF(DH.LT 0.4E-4.OR.ITROT.EQ.0) GO TO 90
      PCP(2) = PCP(2)/(1.+2.*DHSTAR*WM(1)/(TT*(GAMMAS(2)+1.)))
      P(2) = P(1)/PCP(2)
      ITROT = ITROT-1
      GO TO 45
   90 WP(NPT)= WM(1)
      PPP(NPT) = P(IP)
      CPR(NPT)= CPSUM
      K = 0
      IF (TT.LT.(TLOW-150.))GO TO 903
      IF(NC.EQ.0) GO TO 700
      INC = 0
      DO 901 I=1,NS
      IF(IUSE(I).EQ.0.OR.IUSE(I).EQ.-10000) GO TO 901
      INC = INC+1
      IF(EN(I,1).EQ.0.) GO TO 901
      IF (TT.LT.(TEMP(INC,1)-50.).OR.TT.GT.(TEMP(INC,2)+50.))GO TO 903
  901 CONTINUE
  700 IF ( IP.EQ.NP) GO TO 863
      K = NPT
      IF (NPT.NE.13) GO TO 870
      GO TO 863
  903 NPT = NPT - 1
  863 CALL RKTOUT
      IF (NSUB+NSUP.NE.0) CALL RATIO
  865 IF (K.EQ.0) GO TO 1000
      NPT = 2
  870 NPT = NPT + 1
  902 CONTINUE
 1000 RETURN
      END
```

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C                                                                       P1712  01172
      SUBROUTINE HCALC                                                  P1712  01173
C                                                                       P1712  01174
C  CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS                 P1712  01175
C                                                                       P1712  01176
      LOGICAL MOLES                                                     P1712  01177
      DIMENSION NUM(15,5),WS(2)                                         P1712  01178
C                                                                       P1712  01179
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  01180
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  01181
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),3U(15),BOP(15,2)  P1712  01182
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  01183
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  01184
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  01185
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  01186
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  01187
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  01188
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  01189
C                                                                       P1712  01190
      EQUIVALENCE(ANUM,NUM)                                             P1712  01191
C                                                                       P1712  01192
      DATA AG/1HG/,IZERO/2H00/,OX/1HO/                                  P1712  01193
C                                                                       P1712  01194
C  IS TT IN RANGE                                                       P1712  01195
C                                                                       P1712  01196
      IF(TT.LT.(TLOW-100.).OR.TT.GT.(THIGH+1000.))GO TO 80              P1712  01197
      WS(1) = 0.                                                        P1712  01198
      WS(2) = 0.                                                        P1712  01199
      HPP(1)=0.                                                         P1712  01200
      HPP(2)=0.                                                         P1712  01201
      AC(1)=0.                                                          P1712  01202
      AC(2)=0.                                                          P1712  01203
      DO 900 N=1,NREAC                                                  P1712  01204
      K=2                                                               P1712  01205
      IF(FOX(N).EQ.OX)K=1                                               P1712  01206
      PCWT=PECWT(N)                                                     P1712  01207
      IF(MOLES)PCWT=PCWT*RMW(N)                                         P1712  01208
      WS(K) = WS(K) + PCWT                                              P1712  01209
      J = NUM(N,5)                                                      P1712  01210
      IF (J.NE.0) GO TO 90                                              P1712  01211
      DO 10 J=1,L                                                       P1712  01212
      DATA(J)=0.                                                        P1712  01213
   10 CONTINUE                                                          P1712  01214
      DO 40 I=1,4                                                       P1712  01215
      IF(ANUM(N,I).EQ.0.)GO TO 50                                       P1712  01216
      DO 20 J=1,L                                                       P1712  01217
      IF(LLMT(J).EQ.NAME(N,I)) GO TO 30                                 P1712  01218
   20 CONTINUE                                                          P1712  01219
   30 DATA(J)=ANUM(N,I)                                                 P1712  01220
   40 CONTINUE                                                          P1712  01221
   50 IS=0                                                              P1712  01222
      DO 70 J=1,NS                                                      P1712  01223
      IF(IUSE(J).EQ.0)GO TO 55                                          P1712  01224
```

```
      IS = IS+1                                                  P1712  01225
      IF(FAZ(N).EQ.AG)GO TO 70                                   P1712  01226
      IF(TT.LT.TEMP(IS,1).OR.TT.GT.TEMP(IS,2)) GO TO 70          P1712  01227
      GO TO 56                                                   P1712  01228
   55 IF(FAZ(N).NE.AG) GO TO 70                                  P1712  01229
   56 DO 60 I=1,L                                                P1712  01230
      IF(A(I,J).NE.DATA(I))  GO TO 70                            P1712  01231
   60 CONTINUE                                                   P1712  01232
      NUM(N,5) = J                                               P1712  01233
      GO TO 90                                                   P1712  01234
   70 CONTINUE                                                   P1712  01235
      GO TO 80                                                   P1712  01236
   90 NSS = NS                                                   P1712  01237
      NS = J                                                     P1712  01238
      CALL CPHS                                                  P1712  01239
      CPSUM = CPSUM/EN(J,NPT)                                    P1712  01240
      NS = NSS                                                   P1712  01241
      IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.           P1712  01242
      RTEMP(N) = TT                                              P1712  01243
      ENTH(N) = HO(J)*R*TT                                       P1712  01244
      AC(K)=AC(K)+CPSUM*PCWT/RMW(N)                              P1712  01245
  500 HPP(K)=HPP(K)+ENTH(N)*PCWT/RMW(N)                          P1712  01246
  900 CONTINUE                                                   P1712  01247
      DO 950 K=1,2                                               P1712  01248
      IF(HP(K).EQ.0.)GO TO 950                                   P1712  01249
      HPP(K)=HPP(K)/WS(K)                                        P1712  01250
      AC(K)=AC(K)/WS(K)                                          P1712  01251
  950 CONTINUE                                                   P1712  01252
      HSUBO = (WP(1)*HPP(1)+WP(2)*HPP(2))/(WP(1)+WP(2))          P1712  01253
      GO TO 1000                                                 P1712  01254
   80 WRITE(6,85) N                                              P1712  01255
   85 FORMAT(1H0,I2,34HITH REACTANT IS NOT IN THERMO DATA )      P1712  01256
 1000 RETURN                                                     P1712  01257
      END                                                        P1712  01258
```

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            SUBROUTINE MATRIX                                          P1712   01259
      C                                                                P1712   01260
      C                                                                P1712   01261
      C     DOUBLE PRECISION G,X                                       P1712   01262
            LOGICAL HP,SP,TF,IDEBUG,CONVG,NEWR                         P1712   01263
      C                                                                P1712   01264
            COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) P1712  01265
           1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712 01266
           2,TCTN(13)                                                  P1712   01267
            COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150) P1712 01268
           1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)      P1712   01269
            COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) P1712 01270
           1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712 01271
           2 ,PPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)  P1712   01272
           3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712 01273
           4 ,RHOP,RMW(15),TLN,JANF                                    P1712   01274
            COMMON /DOUBLE/ G(20,21), X(20)                            P1712   01275
            COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712 01276
           1  KMAT,IMAT,IQ1,NLJ,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ P1712 01277
           2 ,IONS,AC,NSERT,JSOL,JLIO,KASE(14),NREAC,IC,IQ2            P1712   01278
      C                                                                P1712   01279
            IQ2 = IQ1 + 1                                              P1712   01280
            IQ3 = IQ2 + 1                                              P1712   01281
            KMAT = IQ3                                                 P1712   01282
            IF(.NOT.CONVG.AND.TP) KMAT = IQ2                           P1712   01283
            IMAT = KMAT - 1                                            P1712   01284
      C                                                                P1712   01285
      C     CLEAR MATRIX STORAGES TO ZERO                              P1712   01286
      C                                                                P1712   01287
            DO 211 I=1,IMAT                                            P1712   01288
            DO 211 K=1,KMAT                                            P1712   01289
      C     G(I,K)= 0.0D0                                              P1712   01290
            G(I,K)= 0.0                                                P1712   01291
        211 CONTINUE                                                   P1712   01292
            SSS = 0.                                                   P1712   01293
            HSUM(NPT) = 0.                                             P1712   01294
      C                                                                P1712   01295
      C     BEGIN SET UP OF ITERATION MATRIX                           P1712   01296
      C                                                                P1712   01297
            KK = L                                                     P1712   01298
            DO 65  J=1,NS                                              P1712   01299
            H=H0(J)*EN(J,NPT)                                          P1712   01300
            IF (IUSE(J)) 65,11,70                                      P1712   01301
         11 F = (H0(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)                      P1712   01302
            SS = H-F                                                   P1712   01303
            TERM1 = H                                                  P1712   01304
            IF (KMAT .EQ. IQ2) TERM1 = F                               P1712   01305
            DO 55 I = 1, L                                             P1712   01306
      C                                                                P1712   01307
      C     CALCULATE THE ELEMENTS  R(I,K)                             P1712   01308
      C                                                                P1712   01309
            IF (A(I,J) .EQ. 0.) GO TO 55                               P1712   01310
            TERM= A(I,J)*EN(J,NPT)                                     P1712   01311
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          DO 15  K=I,L                                              P1712  01312
          G(I,K)= G(I,K) + A(K,J)*TERM                              P1712  01313
       15 CONTINUE                                                  P1712  01314
C                                                                   P1712  01315
          G(I,IQ1)=G(I,IQ1)+TERM                                    P1712  01316
          G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1                            P1712  01317
          IF (CONVG .OR.TM) GO TO 55                                P1712  01318
          G(I,IQ3)= G(I,IQ3)+A(I,J)*F                               P1712  01319
          IF (SP) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS                   P1712  01320
       55 CONTINUE                                                  P1712  01321
          IF (KMAT .EQ. IQ2) GO TO 64                               P1712  01322
          IF(CONVG.OR.HP) GO TO 59                                  P1712  01323
          G(IQ2,IQ1) = G(IQ2,IQ1) + SS                              P1712  01324
          G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS                            P1712  01325
          G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F             P1712  01326
          GO TO 62                                                  P1712  01327
       59 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*H                             P1712  01328
          IF (CONVG) GO TO 64                                       P1712  01329
          G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F                             P1712  01330
       62 G(IQ1,IQ3)=G(IQ1,IQ3)+F                                   P1712  01331
       64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM                                P1712  01332
          GO TO 65                                                  P1712  01333
C                                                                   P1712  01334
C   CONDENSED SPECIES                                               P1712  01335
C                                                                   P1712  01336
       70 KK = KK + 1                                               P1712  01337
          DO 75  I = 1,L                                            P1712  01338
          G(I,KK) = A(I,J)                                          P1712  01339
          G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)                  P1712  01340
       75 CONTINUE                                                  P1712  01341
          G(KK,IQ2) = HO(J)                                         P1712  01342
          G(KK,KMAT) = HO(J) - S(J)                                 P1712  01343
          HSUM(NPT) = HSUM(NPT)+ H                                  P1712  01344
          IF(.NOT.SP) GO TO 65                                      P1712  01345
          SSS = SSS + S(J)*EN(J,NPT)                                P1712  01346
          G(IQ2,KK) = S(J)                                          P1712  01347
       65 CONTINUE                                                  P1712  01348
          SSS = SSS + G(IQ2,IQ1)                                    P1712  01349
          HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)                        P1712  01350
          G(IQ1,IQ1) = SUMN - ENN                                   P1712  01351
C                                                                   P1712  01352
C         REFLECT SYMMETRIC PORTIONS OF THE MATRIX                  P1712  01353
C                                                                   P1712  01354
          ISYM = IQ1                                                P1712  01355
          IF(HP.OR.CONVG)ISYM=IQ2                                   P1712  01356
          DO 102 I=1,ISYM                                           P1712  01357
          DO 102 J=I,ISYM                                           P1712  01358
          G(J,I)=G(I,J)                                             P1712  01359
      102 CONTINUE                                                  P1712  01360
C                                                                   P1712  01361
C         COMPLETE THE RIGHT HAND SIDE                              P1712  01362
C                                                                   P1712  01363
          IF(CONVG)  GO TO 175                                      P1712  01364
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            DO 145 I=1,L                                              P1712   01365
            X(1)=B0(I)-G(I,IQ1)                                       P1712   01366
            G(I,KMAT) = G(I,KMAT)+X(1)                                P1712   01367
        145 CONTINUE                                                  P1712   01368
            G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN                        P1712   01369
      C                                                               P1712   01370
      C     COMPLETE ENERGY ROW AND TEMPERATURE COLUMN                P1712   01371
      C                                                               P1712   01372
            IF (KMAT .EQ. IQ2) GO TO 185                              P1712   01373
            IF (SP)ENERGY = S0+ENN-SUMN - SSS                         P1712   01374
            IF(HP)ENERGY=HSUM0/TT - HSUM(NPT)                         P1712   01375
            G(IQ2,IQ3)=G(IQ2,IQ3)+ ENERGY                             P1712   01376
        175 G(IQ2,IQ2)= G(IQ2,IQ2)+CPSUM                              P1712   01377
        185 RETURN                                                    P1712   01378
            END                                                       P1712   01379
```

```
      SUBROUTINE MGAUSO                                                 P1712 01380
C                                                                       P1712 01381
C     SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS                        P1712 01382
C                                                                       P1712 01383
C     DOUBLE PRECISION G,X,COEFX(20),SUM,Z                              P1712 01384
      DIMENSION COEFX(20)                                               P1712 01385
C                                                                       P1712 01386
      COMMON/COUBLE/G(20,21),X(20)                                      P1712 01387
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPI,L,NS, P1712 01388
     1  KMAT,IMAT,IO1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712 01389
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IO2                   P1712 01390
C                                                                       P1712 01391
      EQUIVALENCE (IUSE,IMAT)                                           P1712 01392
C                                                                       P1712 01393
      DATA BIGNO/1.E+38/                                                P1712 01394
C                                                                       P1712 01395
C     BEGIN ELIMINATION OF NNTH VARIABLE                                P1712 01396
C                                                                       P1712 01397
      IUSE1=IUSE+1                                                      P1712 01398
    6 DO 45 NN=1,IUSE                                                   P1712 01399
      IF (NN-IUSE) 8,83,5                                               P1712 01400
   83 IF(G(NN,NN))31,23,31                                              P1712 01401
C                                                                       P1712 01402
C     SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW                        P1712 01403
C                                                                       P1712 01404
    8 DO 18 I=NN,IUSE                                                   P1712 01405
      COEFX(I) = BIGNO                                                  P1712 01406
      IF(G(I,NN).EQ.0.)  GO TO 18                                       P1712 01407
      COEFX(I) = 0.                                                     P1712 01408
      DO 10 J=NN,IUSE1                                                  P1712 01409
      SUM = G(I,J)                                                      P1712 01410
      IF(SUM.LT.0.)  SUM=-SUM                                           P1712 01411
      IF(J.NE.NN)  GO TO 9                                              P1712 01412
      Z = SUM                                                           P1712 01413
      GO TO 10                                                          P1712 01414
    9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM                                 P1712 01415
   10 CONTINUE                                                          P1712 01416
      COEFX(I) = COEFX(I)/Z                                             P1712 01417
   18 CONTINUE                                                          P1712 01418
      TEMP = BIGNO                                                      P1712 01419
      I=0                                                               P1712 01420
   20 DO 22 J=NN,IUSE                                                   P1712 01421
      IF (COEFX(J)-TEMP) 87,22,22                                       P1712 01422
   87 TEMP=COEFX(J)                                                     P1712 01423
      I=J                                                               P1712 01424
   22 CONTINUE                                                          P1712 01425
      IF(I) 28,23,28                                                    P1712 01426
C                                                                       P1712 01427
C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH       P1712 01428
C     VARIABLE FROM THE REMAINING EQUATIONS                             P1712 01429
C                                                                       P1712 01430
C      INTERCHANGE EQUATIONS I AND NN                                   P1712 01431
C                                                                       P1712 01432
```

```
      28 IF(NN-I) 29,31,29                                     P1712  01433
      29 DO 30 J=NN,IUSE1                                      P1712  01434
         Z=G(I,J)                                              P1712  01435
         G(I,J)=G(NN,J)                                        P1712  01436
         G(NN,J)=Z                                             P1712  01437
      30 CONTINUE                                              P1712  01438
C                                                              P1712  01439
C        DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH    P1712  01440
C        VARIABLE FROM THE REMAINING EQUATIONS                 P1712  01441
C                                                              P1712  01442
      31 K = NN + 1                                            P1712  01443
         DO 36 J = K, IUSE1                                    P1712  01444
         IF(G(NN,NN).EQ.0.)  GO TO 23                          P1712  01445
            G(NN,J) = G(NN,J) / G(NN,NN)                       P1712  01446
      36 CONTINUE                                              P1712  01447
         IF(K-IUSE1) 38,45,38                                  P1712  01448
      38 DO 44 I = K,IUSE                                      P1712  01449
      40 DO 44 J = K, IUSE1                                    P1712  01450
            G(I,J) = G(I,J) - G(I,NN)*G(NN,J)                  P1712  01451
      44 CONTINUE                                              P1712  01452
      45 CONTINUE                                              P1712  01453
C                                                              P1712  01454
C        BACKSOLVE FOR THE VARIABLES                           P1712  01455
C                                                              P1712  01456
         K = IUSE                                              P1712  01457
      47 J = K + 1                                             P1712  01458
C        X(K) = 0.000                                          P1712  01459
         X(K) = 0.0                                            P1712  01460
         SUM = 0.0                                             P1712  01461
         IF(IUSE - J) 51,48,48                                 P1712  01462
      48 DO 50 I = J,IUSE                                      P1712  01463
            SUM = SUM + G(K,I)* X(I)                           P1712  01464
      50 CONTINUE                                              P1712  01465
      51 X(K) = G(K,IUSE1) - SUM                               P1712  01466
         K = K - 1                                             P1712  01467
         IF (K) 67,151,47                                      P1712  01468
      23 IUSE = IUSE-1                                         P1712  01469
     151 RETURN                                                P1712  01470
         END                                                   P1712  01471
```

```
      SUBROUTINE MOLIER
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)
     2,TCTN(13)
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
     1 ,DELN(150),A(15,150),SUM(150,3),IUSE(150),TEMP(50,2)
      COMMON/MISC/ERN,SUMN,TT,SU,ATOM(3,101),LLMT(15),BU(15),BOP(15,2)
     1 ,TK,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
     4 ,RHOP,RMW(15),TLN,JANF
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSF,IPSP,MOLES,NP,NT,NPT,L,NS,
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
     2 ,IONS,KC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,YO2
      DO 91 IT = 1,26
      IF (T(IT).EQ. 0.) GO TC 95
      NT = IT
   91 CONTINUE
C
C     SET ASSIGNED P
C
   95 DO 902 IP = 1,NP
      PP = P(IP)
C
C     SET ASSIGNED T
C
      DO 902 IT=1,NT
      TT = T(IT)
      CALL EQLBRM
      IF(TT.NE.0.)  GO TO 908
      IF(NPT.EQ.1)  GO TO 1000
  800 K = 0
      IF(IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.)  GO TO 860
      K = NPT
      IF(NPT.NE.13)  GO TO 870
  860 WRITE (6,5)
    5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
     1     ,/43X,28H TEMPERATURES AND PRESSURES     ///  )
      CALL OUT1
      WRITE (6,863)
  863 FORMAT (25HOTHERMODYNAMIC PROPERTIES//)
      CALL OUT2
      CALL OUT3
  865 IF(K.EQ.0) GO TO 1000
      WRITE(6,868)
  868 FORMAT(1H1)
      NPT = 0
  870 NPT = NPT + 1
C
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
C
      DO 880 I = 1,NS
```

```
            EN(I,NPT) = EN(I,K)                                          P1712  01525
        880 CONTINUE                                                     P1712  01526
        902 CONTINUE                                                     P1712  01527
       1000 RETURN                                                       P1712  01528
            END                                                          P1712  01529
```

SUBROUTINE OUT1 FORTRAN EXTENDED VERSION 2.0 31/12/70 08.09.56. PAGE NO. 1

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      SUBROUTINE OUT1                                                  P1712  01530
C                                                                      P1712  01531
C     DOUBLE PRECISION G,X                                             P1712  01532
      LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,MOLES                       P1712  01533
C                                                                      P1712  01534
      DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5)                    P1712  01535
C                                                                      P1712  01536
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      P1712  01537
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712  01538
     2  ,TOTN(13)                                                      P1712  01539
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712  01540
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712  01541
      COMMON/MISC/ENN,SUMN,TT,SU,ATOM(3,101),LLMT(15),BO(15),BOP(15,2) P1712  01542
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AL(2),AM(2) P1712  01543
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712  01544
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  01545
     4 ,RHCP,FMW(15),TLN,JANF                                          P1712  01546
      COMMON /DOUBLE/ G(20,21), X(20)                                  P1712  01547
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  01548
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712  01549
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712  01550
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  01551
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSG                            P1712  01552
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)    P1712  01553
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2       P1712  01554
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FD                      P1712  01555
      COMMON/CVOLUM/ VOLUMC,IMPETUS,IFLGGG                             P1712  01556
      COMMON/PRCENT/ FMULE                                             P171201 00001
      REAL IMPETUS                                                     P1712  01557
C                                                                      P1712  01558
      EQUIVALENCE (V,NV),(Z,H0)                                        P1712  01559
C                                                                      P1712  01560
C     HEAD=(1H ,2A4,5  (A2,F8.5,3X),5  X,F7.5,F13.3,4X,A1,F10.2,F9.4)  P1712  01561
C                                                                      P1712  01562
      DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX,    P1712  01563
     1    ,4HF7.5 ,4H,F13 ,4H.3,4 ,4HX,A1 ,4H,F10 ,4H.2,F ,4H9.4)/     P1712  01564
      DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/                P1712  01565
     1        ,YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /                       P1712  01566
     2        ,YX/3H,57,3H,44,3H,31,3H,18,2H,5 /                       P1712  01567
C                                                                      P1712  01568
      WRITE(6,4) KASE                                                  P1712  01569
    4 FORMAT(1H0,13A6,A2)                                              P1712  01570
    3 FORMAT (9H CASE NO. ,I5)                                         P1712  01571
      IF(.NOT.MOLES) WRITE(6,5)                                        P1712  01572
    5 FORMAT (77X,46HWT FRACTION  ENTHALPY  STATE   TEMP    DENSITY/   P1712  01573
     1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE)     CAL/MOL,10X,5HDEG K, P1712  01574
     2 4X,4HG/CC )                                                     P1712  01575
      IF(MOLES) WRITE(6,6)                                             P1712  01576
    6 FORMAT (84X,5HMOLES,8X,   33HENTHALPY  STATE    TEMP    DENSITY/ P1712  01577
     1 10X,16HCHEMICAL FORMULA,67X,7HCAL/MOL,10X,13HDEG K     G/CC )   P1712  01578
      DO 15 N=1,NREAC                                                  P1712  01579
      IF(FOX(N).EQ.FOX(N-1))GO TO 11                                   P1712  01580
      IF(FOX(N).NE.OX)GO TO 10                                         P1712  01581
```

```
      HO1 = CXIO                                                   P1712  01582
      HO2 = ANT                                                    P1712  01583
      GO TO 11                                                     P1712  01584
   10 HO1 = FUEL                                                   P1712  01585
      HO2 = F8                                                     P1712  01586
   11 DO 13 J=1,5                                                  P1712  01587
      IF(ANUM(N,J).EQ.0.)GO TO 14                                  P1712  01588
   13 CONTINUE                                                     P1712  01589
      J=6                                                          P1712  01590
   14 J=J-1                                                        P1712  01591
      HEAD(3)=YN(J)                                                P1712  01592
      HEAD(7)=YX(J)                                                P1712  01593
      WRITE(6,HEAD)HO1,HO2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECNT(N),ENTH(P1712  01594
     1N), FAZ(N),RTEMP(N),DENS(N)                                  P1712  01595
   15 CONTINUE                                                     P1712  01596
      WRITE(6,20) OF,FPCT,EQRAT,RHOP                               P1712  01597
   20 FORMAT (1H0,15X, 4HO/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,   P1712  01598
     1  19HEQUIVALENCE RATIO= ,F7.4,4X,8HDENSITY=,F8.4//)          P1712  01599
C                                                                  P1712  01600
      AGV = 9.80665                                                P1712  01601
      DO 25 I = 1,NPT                                              P1712  01602
      TOTN(I) = 0                                                  P1712  01603
      DO 25 J = 1,NS                                               P1712  01604
      TOTN(I) = TOTN(I) + EN(J,I)                                  P1712  01605
   25 CONTINUE                                                     P1712  01606
      FMT(4)= FMT(6)                                               P1712  01607
      RETURN                                                       P1712  01608
C                                                                  P1712  01609
      ENTRY OUT2                                                   P1712  01610
C                                                                  P1712  01611
C   PRESSURE                                                       P1712  01612
C                                                                  P1712  01613
      DO 55 I=1,NPT                                                P1712  01614
      K= 2*I+3                                                     P1712  01615
      FMT(K)= F4                                                   P1712  01616
      IF (PPP(I).GE.1.) FMT(K)=F3                                  P1712  01617
      IF (PPP(I).GE.10.) FMT(K)=F2                                 P1712  01618
      IF (PPP(I).GE.100.) FMT(K)=F1                                P1712  01619
   55 CONTINUE                                                     P1712  01620
      WRITE (6,FMT)(FP(I),I=1,4),(PPP(J),J=1,NPT)                  P1712  01621
C                                                                  P1712  01622
C   TEMPERATURE                                                    P1712  01623
C                                                                  P1712  01624
      DO 65 I=1,NPT                                                P1712  01625
      NV(I)= TT(I)+.5                                              P1712  01626
   65 CONTINUE                                                     P1712  01627
      FMT(4)= FMT13                                                P1712  01628
      FMT(5)= FMT19                                                P1712  01629
      WRITE (6,FMT)(FT(I),I=1,4),(NV(J),J=1,NPT)                   P1712  01630
C                                                                  P1712  01631
C   ENTHALPY                                                       P1712  01632
C                                                                  P1712  01633
      DO 75 I=1,NPT                                                P1712  01634
```

```
      V(I) = HSUM(I) * R
   75 CONTINUE
      FMT(5)= FB
      FMT(7)= F1
      WRITE (6,FMT)(FH(I),I=1,4),(V(J),J=1,NPT)
C
C  ENTROPY
C
      FMT(7)=F4
      DO 78 I = 1,NPT
      V(I) = SSUM(I) * R
   78 CONTINUE
      WRITE (6,FMT)(FS(I),I=1,4),(V(J),J=1,NPT)
      WRITE (6,80)
   80 FORMAT ( 1H )
C
C  MOLECULAR WEIGHT
C
      FMT(7)= F3
      WRITE (6,FMT)(FM(I),I=1,4),(WM(J),J=1,NPT)
C
C  (DLV/DLP)T
C
      FMT(7)=F5
      IF(EQL) WRITE(6,FMT)(FV(I),I=1,4),(DLVPT(J),J=1,NPT)
C
C  (DLV/DLT)P
C
      FMT(7)= F4
      IF(EQL) WRITE(6,FMT)(FD(I),I=1,4),(DLVTP(J),J=1,NPT)
C
C  HEAT CAPACITY
C
      DO 85  I=1,NPT
      V(I) = CPR(I) * R
   85 CONTINUE
      WRITE(6,FMT)(FC(I),I=1,4),(V(J),J=1,NPT)
C
C  GAMMA(S)
C
      WRITE(6,FMT)(FG(I),I=1,4),(GAMMAS(J),J=1,NPT)
C
C  SONIC VELOCITY
C
      FMT(7)= F1
      DO 95 I = 1,NPT
      SONVEL(I) = SQRT(RR*GAMMAS(I)*TTT(I)/WM(I))
   95 CONTINUE
      WRITE(6,FMT)(FL(I),I=1,4),(SONVEL(J),J=1,NPT)
      VOLUMC=GAMMAS(1)*TTT(1)
      IMPETUS=VOLUMC*2781./WM(1)
      RETURN
C
```

```
         ENTRY OUT3                                                    P1712   01688
         IF(.NOT.EQL)  GO TO 331                                       P1712   01689
C                                                                      P1712   01690
C    MOLE FRACTIONS - EQUILIBRIUM                                      P1712   01691
C                                                                      P1712   01692
         WRITE (6,80)                                                  P1712   01693
         FMT(7)= F9                                                    P1712   01694
         WRITE(6,310)                                                  P1712   01695
     310 FORMAT(15H0MOLE FRACTIONS //)                                 P1712   01696
         DO 330 K=1,NS                                                 P1712   01697
         DO 315 I=1,NPT                                                P1712   01698
         V(I) = EN(K,I) /TOTN(I)                                       P1712   01699
     315 CONTINUE                                                      P1712   01700
         DO 316 I=1,NPT                                                P1712   01701
         IF (V(I).GE.(5.E-6)) GO TO 320                                P1712   01702
     316 CONTINUE                                                      P1712   01703
         GO TO 330                                                     P1712   01704
     320 WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT)    P1712   01705
     330 CONTINUE                                                      P1712   01706
     331 WRITE(6,335)                                                  P1712   01707
     335 FORMAT(113H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MO P1712   01708
        1LE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS//) P1712   01709
         LINE= 0                                                       P1712   01710
         DO 350 K=1,NS                                                 P1712   01711
         DO 340 I=1,NPT                                                P1712   01712
         IF ((EN(K,I)/TOTN(I)).GE.(5.E-6)) GO TO 343                   P1712   01713
     340 CONTINUE                                                      P1712   01714
         LINE= LINE+1                                                  P1712   01715
         Z(LINE,1)= SUB(K,1)                                           P1712   01716
         Z(LINE,2)= SUB(K,2)                                           P1712   01717
         Z(LINE,3)= SUB(K,3)                                           P1712   01718
     343 IF ((LINE.NE.10) .AND. K.NE.NS) GO TO 350                     P1712   01719
         IF (LINE.EQ.0) GO TO 1000                                     P1712   01720
         WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)              P1712   01721
     345 FORMAT (10(1X,3A4))                                           P1712   01722
         LINE= 0                                                       P1712   01723
     350 CONTINUE                                                      P1712   01724
         IF(.NOT.MOLES) WRITE(6,360)                                   P1712   01725
     360 FORMAT(78H0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXI P1712   01726
        2DANT IN TOTAL OXIDANTS    )                                   P1712   01727
         WRITE(6,1100) PMOLE                                           P171201 00002
    1100 FORMAT(1H0,*VISCOSITY AND CONDUCTIVITY VALUES BASED ON *,F5.1,* PE P171201 00003
        1RCENT OF GAS MIXTURE*)                                        P171201 00004
    1000 RETURN                                                        P1712   01728
         END                                                           P1712   01729
```

```
      SUBROUTINE RATIO                                                  P1712   01730
C                                                                       P1712   01731
C     (USED FOR AREA RATIO INTERPOLATION ONLY)                          P1712   01732
C                                                                       P1712   01733
C     DOUBLE PRECISION G,X                                              P1712   01734
      LOGICAL EQL, FROZ,TPSP                                            P1712   01735
C                                                                       P1712   01736
      DIMENSION PER(2,2),AI(13),APCP(13),AT(13),AMWT(13),RP(2),NV(13)   P1712   01737
     1 , RPP(2)                                                         P1712   01738
C                                                                       P1712   01739
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712   01740
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)  P1712   01741
     2,TCTN(13)                                                         P1712   01742
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712   01743
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712   01744
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),BU(15),BOP(15,2)  P1712   01745
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712   01746
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712   01747
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712   01748
     4 ,RHOP,KMW(15),TLN,JANF                                           P1712   01749
      COMMON /DOUBLE/ G(20,21), X(20)                                   P1712   01750
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712   01751
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712   01752
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),JREAC,IC,IQ2                   P1712   01753
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712   01754
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SS0                             P1712   01755
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)     P1712   01756
     1  ,FC(4),FG(4),F8,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2        P1712   01757
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                       P1712   01758
C                                                                       P1712   01759
      EQUIVALENCE (V,NV)                                                P1712   01760
C                                                                       P1712   01761
      NBLO = NPT-2                                                      P1712   01762
      DO 22 J=3,NPT                                                     P1712   01763
      IF(PCP(J).GT.PCP(2))GO TO 30                                      P1712   01764
   22 CONTINUE                                                          P1712   01765
      GO TO 31                                                          P1712   01766
   30 NBLO=J-3                                                          P1712   01767
   31 DO 1200  ISONIC=1,2                                               P1712   01768
      LL = 1                                                            P1712   01769
      IF(ISONIC.EQ.2)  GO TO 34                                         P1712   01770
      IF(NSUB.EQ.0)  GO TO 1200                                         P1712   01771
      NAR = NSUB                                                        P1712   01772
      GO TO 36                                                          P1712   01773
   34 IF(NSUP.EQ.0)  GO TO 1200                                         P1712   01774
      NAR = NSUP                                                        P1712   01775
   36 DO 1100 I=1,NAR                                                   P1712   01776
      IF(ISONIC.EQ.2)  GO TO 40                                         P1712   01777
      IF(NBLO.LE.1) GO TO 1100                                          P1712   01778
      K=2+NBLO                                                          P1712   01779
      DO 38 JJ=4,K                                                      P1712   01780
      J=JJ                                                              P1712   01781
      V(LL) = SUBAR(I)                                                  P1712   01782
```

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      IF(V(LL).GE.AEAT(J))  GO TO 56                    P1712  01783
   38 CONTINUE                                          P1712  01784
      GO TO 56                                          P1712  01785
   40 IF(NPT-NBLO.LE.3)   GO TO 1100                    P1712  01786
      V(LL) = SUPAR(I)                                  P1712  01787
      K=4+NBLO                                          P1712  01788
      DO 42 JJ=K,NPT                                    P1712  01789
      J=JJ                                              P1712  01790
      IF(V(LL).LE.AEAT(J))   GO TO 56                   P1712  01791
   42 CONTINUE                                          P1712  01792
      IF(V(LL).GE.AEAT(J)*3.)   GO TO 85                P1712  01793
   56 KJ = J-1                                          P1712  01794
      K = KJ                                            P1712  01795
      DO 64 JJ=1 2                                      P1712  01796
      IF(CPR(K).NE.0.)   GO TO 63                       P1712  01797
      WRITE(6,62)K                                      P1712  01798
   62 FORMAT(17HOCANNOT USE POINT,I2,3X,4HCP=0 )        P1712  01799
      GO TO 1100                                        P1712  01800
   63 PER(JJ,1)=-1./(CPR(K)*WM(K))                      P1712  01801
      IF (EQL) PER(JJ,1) =  PER(JJ,1)*DLVTP(K)          P1712  01802
      PER(JJ,2)=    TTT(K)/(2.*WM(K)*(HSUM(1)-HSUM(K))) P1712  01803
      RP(JJ) = 1./(1./GAMMAS(K)-PER(JJ,2))              P1712  01804
      IF(EQL)RPP(JJ) = 1.+DLVPT(K)+(1.-DLVTP(K))*PER(JJ,1)  P1712  01805
      K = KJ + 1                                        P1712  01806
   64 CONTINUE                                          P1712  01807
      AMWT(LL) = WM(1)                                  P1712  01808
      CALL SET(PCP(KJ),RP(1),AEAT(KJ),V(LL),   APCP(LL))  P1712  01809
      CALL SET(TTT(KJ),PER(1,1),PCP(KJ),APCP(LL),AT(LL))  P1712  01810
      IF(EQL)CALL SET (WM(KJ),RPP(1),PCP(KJ),APCP(LL),AMWT(LL))  P1712  01811
      K = KJ                                            P1712  01812
      DO 74 JJ=1,2                                      P1712  01813
      G(JJ,7)=SPIM(K)**2                                P1712  01814
      G(JJ+2,7)=2.*G(JJ,7)*PER(JJ,2)                    P1712  01815
      G(JJ+4,7)=(1.-GAMMAS(K))/GAMMAS(K)*G(JJ+2,7)      P1712  01816
      G(JJ,1)=1.                                        P1712  01817
      G(JJ+2,1)= 0                                      P1712  01818
      G(JJ+4,1)=0                                       P1712  01819
      G(JJ,2)=ALOG(PCP(K))                              P1712  01820
      G(JJ+2,2)=1.                                      P1712  01821
      G(JJ+4,2)=0                                       P1712  01822
      DO 70 M=3,6                                       P1712  01823
      MXP=M-1                                           P1712  01824
      G(JJ,M)=G(JJ,2)**MXP                              P1712  01825
      MXP=MXP-1                                         P1712  01826
      G(JJ+2,M)=G(JJ,2)**MXP*FLOAT(M-1)                 P1712  01827
      G(JJ+4,M)=G(JJ+2,M)/G(JJ,2)*FLOAT(M-2)            P1712  01828
   70 CONTINUE                                          P1712  01829
      K = KJ + 1                                        P1712  01830
   74 CONTINUE                                          P1712  01831
      IMAT = 6                                          P1712  01832
      CALL MGAUSD                                       P1712  01833
      AI(LL)= X (1)                                     P1712  01834
      DO 84 JJ=2,6                                      P1712  01835
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```
      AI(LL)=AI(LL)+ X (JJ)*ALOG(APCP(LL))**(JJ-1)        P1712   01836
   84 CONTINUE                                            P1712   01837
      IF(AI(LL).LE.0.)GO TO 85                            P1712   01838
      AI(LL) = AI(LL)**.5                                 P1712   01839
      GO TO 86                                            P1712   01840
   85 LL = LL - 1                                         P1712   01841
   86 IF(LL.GE.15.OR.I.GE.NAR) GO TO 90                   P1712   01842
      LL = LL+1                                           P1712   01843
      GO TO 1100                                          P1712   01844
C                                                         P1712   01845
C     OUTPLT                                              P1712   01846
C                                                         P1712   01847
   90 IF(EQL) WRITE (6,87)                                P1712   01848
   87 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING E P171201 00005
     1QUILIBRIUM COMPOSITION DURING EXPANSION*//)         P1712   01850
      IF (.NOT.EQL) WRITE (6,88)                          P1712   01851
   88 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING F P171201 00006
     1ROZEN COMPOSITION DURING EXPANSION*//)              P1712   01853
      IF (TPSM) WRITE (6,99)                              P1712   01854
   99 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE       )   P1712   01855
      WRITE (6,91)                                        P1712   01856
   91 FORMAT (52X,24HFOR ASSIGNED AREA RATIOS     //)     P1712   01857
      PC= P(1)*14.696E06                                  P1712   01858
      WRITE(6,191)PC                                      P1712   01859
  191 FORMAT(5H P  = ,F8.1,5H PSIA)                       P1712   01860
      CALL OUT1                                           P1712   01861
      IF(ISONIC.EQ.1) WRITE(6,33)                         P1712   01862
   33 FORMAT(18H0SUBSONIC FLOW      //)                   P1712   01863
      IF (ISONIC.EQ.2) WRITE (6,35)                       P1712   01864
   35 FORMAT(18H0SUPERSONIC FLOW    //)                   P1712   01865
C                                                         P1712   01866
C     AREA RATIO                                          P1712   01867
C                                                         P1712   01868
      FMT(6)= FMT(8)                                      P1712   01869
      FMT(4)= FMT(6)                                      P1712   01870
      DO 92 M=1,LL                                        P1712   01871
      K= 2*M+3                                            P1712   01872
      FMT(K)= F3                                          P1712   01873
      IF(V(M).GE.10.) FMT(K)=F2                           P1712   01874
      IF(V(M).GE.100.) FMT(K)=F1                          P1712   01875
   92 CONTINUE                                            P1712   01876
      WRITE(6,FMT) FA1,FA2,FB,FB,(V(M),M=1,LL)            P1712   01877
C                                                         P1712   01878
C     VACUUM SPECIFIC IMPULSE AND SPECIFIC IMPULSE        P1712   01879
C                                                         P1712   01880
      DO 93 M=1,LL                                        P1712   01881
      V(M)=AI(M)+CSTR*V(M)/(32.174* APCP(M))              P1712   01882
   93 CONTINUE                                            P1712   01883
      FMT(4)= FMT13                                       P1712   01884
      FMT(5)= F8                                          P1712   01885
      FMT(7)= F1                                          P1712   01886
      WRITE(6,FMT) (FA(N),N=1,4), (V(M),M=1,LL)           P1712   01887
      WRITE(6,FMT) (FI(N),N=1,4), (AI(M),M=1,LL)          P1712   01888
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      C                                                  P1712   01889
      C     C*                                           P1712   01890
      C                                                  P1712   01891
            FMT(5)= FMT19                                P1712   01892
            DO 94 M=1,LL                                 P1712   01893
            NV(M)=CSTR +.5                               P1712   01894
         94 CONTINUE                                     P1712   01895
            WRITE(6,FMT) (FR(N),N=1,4), (NV(M),M=1,LL)   P1712   01896
      C                                                  P1712   01897
      C     CF - THRUST COEFFICIENT                      P1712   01898
      C                                                  P1712   01899
            DO 95 M=1,LL                                 P1712   01900
            V(M)=AI(M)*32.174/CSTR                       P1712   01901
         95 CONTINUE                                     P1712   01902
            FMT(5)= F8                                   P1712   01903
            FMT(7)= F3                                   P1712   01904
            WRITE(6,FMT) FC1,F8,F8,F8,(V(M),M=1,LL)      P1712   01905
            WRITE(6,96)                                  P1712   01906
         96 FORMAT(1H )                                  P1712   01907
      C                                                  P1712   01908
      C     PRESSURE RATIO                               P1712   01909
      C                                                  P1712   01910
            FMT(4)= FMT(6)                               P1712   01911
            DO 97 M=1,LL                                 P1712   01912
            K= 2*M+3                                     P1712   01913
            FMT(K)= F3                                   P1712   01914
            IF(APCP(M).GE.1000.) FMT(K)=F2               P1712   01915
            IF(APCP(M).GE.10000.) FMT(K)=F1              P1712   01916
         97 CONTINUE                                     P1712   01917
      C                                                  P1712   01918
      C     PRESSURE                                     P1712   01919
      C                                                  P1712   01920
            WRITE(6,FMT) FR1,F8,F8,F8,(APCP(M),M=1,LL)   P1712   01921
            DO 98 M=1,LL                                 P1712   01922
            K= 2*M+3                                     P1712   01923
            V(M)=P(1)/APCP(M)                            P1712   01924
            FMT(K)= F4                                   P1712   01925
            IF(V(M).GE.1.) FMT(K)=F3                     P1712   01926
            IF(V(M).GE.10.) FMT(K)=F2                    P1712   01927
            IF(V(M).GE.100.) FMT(K)=F1                   P1712   01928
         98 CONTINUE                                     P1712   01929
            WRITE(6,FMT) (FP(N),N=1,4), (V(M),M=1,LL)    P1712   01930
      C                                                  P1712   01931
      C     TEMPERATURE                                  P1712   01932
      C                                                  P1712   01933
            DO 101 M=1,LL                                P1712   01934
            NV(M)=AT(M)+.5                               P1712   01935
        101 CONTINUE                                     P1712   01936
            FMT(4)= FMT13                                P1712   01937
            FMT(5)= FMT19                                P1712   01938
            WRITE(6,FMT) (FT(N),N=1,4), (NV(M),M=1,LL)   P1712   01939
      C                                                  P1712   01940
      C     ENTHALPY                                     P1712   01941
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                                                        P1712  01942
      C                                                 P1712  01943
            FMT(5)= F8                                  P1712  01944
            FMT(7)= F1                                  P1712  01945
            DO 104 M=1,LL                               P1712  01946
            V(M)= MSUM(1)*R-1000.*(AI(M)/294.98)**2     P1712  01947
        104 CONTINUE                                    P1712  01948
            WRITE(6,FMT) (FM(N),N=1,4), (V(M),M=1,LL)   P1712  01949
      C                                                 P1712  01950
      C     ENTROPY                                     P1712  01951
      C                                                 P1712  01952
            FMT(7)=F4                                   P1712  01953
            V(1) = SSUM(2)*R                            P1712  01954
            DO 106 M=1,LL                               P1712  01955
            V(M) = V(1)                                 P1712  01956
        106 CONTINUE                                    P1712  01957
            WRITE(6,FMT) (FS(N),N=1,4), (V(M),M=1,LL)   P1712  01958
      C                                                 P1712  01959
      C     MOLECULAR WEIGHT                            P1712  01960
      C                                                 P1712  01961
            FMT(7)=F3                                   P1712  01962
            WRITE(6,FMT) (FM(N),N=1,4), (AMWT(M),M=1,LL) P1712  01963
       1100 CONTINUE                                    P1712  01964
       1200 CONTINUE                                    P1712  01965
            RETURN                                      P1712  01966
            END
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      SUBROUTINE REACT                                                  P1712 01967
C                                                                       P1712 01968
C                                                                       P1712 01969
C     DOUBLE PRECISION G,X                                              P1712 01970
      LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR,IONS,MOLES,EQL,FROZ            P1712 01971
C                                                                       P1712 01972
      DIMENSION ANAME(15,5),V(15)                                       P1712 01973
C                                                                       P1712 01974
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712 01975
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,MSUB0,AC(2),AM(2) P1712 01976
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712 01977
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712 01978
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712 01979
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712 01980
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712 01981
     2 ,IONS,KC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712 01982
C                                                                       P1712 01983
      EQUIVALENCE (NAME,ANAME)                                          P1712 01984
C                                                                       P1712 01985
      DATA MOL/1HM/,OX/1HO/,LANK/1H /,IZERO/2H00/                       P1712 01986
C                                                                       P1712 01987
      WRITE(6,9000)                                                     P1712 01988
 9000 FORMAT(1H ,*REACTANTS*)                                           P1712 01989
      DO 10 K=1,2                                                       P1712 01990
      WP(K)=0.                                                          P1712 01991
      HPP(K)=0.                                                         P1712 01992
      RHO(K)=0.                                                         P1712 01993
      VPLS(K)=0.                                                        P1712 01994
      VMIN(K)=0.                                                        P1712 01995
      AC(K)=0.                                                          P1712 01996
      AM(K)=0.                                                          P1712 01997
      DO 8 J=1,15                                                       P1712 01998
      LLMT(J)=0                                                         P1712 01999
      B0P(J,K)=0.                                                       P1712 02000
    8 CONTINUE                                                          P1712 02001
   10 CONTINUE                                                          P1712 02002
      N=1                                                               P1712 02003
      L=1                                                               P1712 02004
      NREACS=NREAC                                                      P1712 02005
      IF(NREAC.GT.16) NREAC=16                                          P1712 02006
      DO 200 N=1,NREAC                                                  P1712 02007
   20 READ(5,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N) P1712 02008
     1 ,RTEMP(N),FOX(N),DENS(N)                                         P1712 02009
   21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F8.5,A1,F8.5)                   P1712 02010
      IF(NAME(N,1).EQ.LANK) GO TO 200                                   P1712 02011
      IF(L.EQ.0)GO TO 20                                                P1712 02012
      WRITE (6,31)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ P1712 02013
     1  (N),RTEMP(N),FOX(N),DENS(N)                                     P1712 02014
   31 FORMAT(1X,5(A2,1X,F7.4,2X),F9.4,2X,A1,F11.2,2X,A1,2X,F8.3,2X,     P1712 02015
     1A1,3X,F8.5)                                                       P1712 02016
   35 IF(MOLE.EQ.MOL) MOLES=.TRUE.                                      P1712 02017
      K=2                                                               P1712 02018
      IF(FOX(N).EQ.OX)K=1                                               P1712 02019
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      DO 38 J=1,15                                              P1712   02020
      DATA(J) = 0.                                              P1712   02021
   38 CONTINUE                                                  P1712   02022
      RM=0.                                                     P1712   02023
      GO 100 JJ=1,5                                             P1712   02024
      IF(ANUM(N,JJ).EQ.0.)GO TO 101                             P1712   02025
      DO 41 J=1,15                                              P1712   02026
      NJ = J                                                    P1712   02027
      IF(LLMT(J).EQ.0) GO TO 45                                 P1712   02028
      IF(NAME(N,JJ).EQ.LLMT(J))GO TO 46                         P1712   02029
   41 CONTINUE                                                  P1712   02030
   45 L = NJ                                                    P1712   02031
      LLMT(J)=NAME(N,JJ)                                        P1712   02032
   46 DO 48 KK=1,101                                            P1712   02033
      IF(ATOM(1,KK).EQ.ANAME(N,JJ))GO TO 50                     P1712   02034
   48 CONTINUE                                                  P1712   02035
      L=0                                                       P1712   02036
      GO TO 20                                                  P1712   02037
   50 RM=RM+ANUM(N,JJ)*ATOM(2,KK)                               P1712   02038
      V(J)=ATOM(3,KK)                                           P1712   02039
      DATA(J)=ANUM(N,JJ)                                        P1712   02040
  100 CONTINUE                                                  P1712   02041
  101 PCNT=PECNT(N)                                             P1712   02042
      IF(MOLES) PCNT=PCNT*RM                                    P1712   02043
      WP(K)=WP(K) + PCNT                                        P1712   02044
      IF(NAME(N,5).NE.IZERO)HPP(K)=HPP(K)+ENTH(N)*PCNT/RM       P1712   02045
      AM(K)=AM(K)+PCNT/RM                                       P1712   02046
      DO 110  J=1,L                                             P1712   02047
      BOP(J,K)=DATA(J)*PCNT/RM +BOP(J,K)                        P1712   02048
  110 CONTINUE                                                  P1712   02049
      IF(DENS(N).NE.0.)GO TO 115                                P1712   02050
      GO TO 117                                                 P1712   02051
  115 RHO(K)=RHO(K)+PCNT/DENS(N)                                P1712   02052
  117 RMK(N) = RM                                               P1712   02053
  200 CONTINUE                                                  P1712   02054
      IF(NREACS.LE.16) GO TO 1205                               P1712   02055
      NRAC=NREACS-16                                            P1712   02056
      DO 1200 I=1,NRAC                                          P1712   02057
 1200 READ(5,21) JUNK                                           P1712   02058
 1205 IF(L.EQ.0) GO TO 1000                                     P1712   02059
      IF(L.EQ.0) GO TO 1000                                     P1712   02060
      DO 220 K=1,2                                              P1712   02061
      IF(WP(K).EQ.0.)GO TO 220                                  P1712   02062
      HPP(K)=HPP(K)/WP(K)                                       P1712   02063
      AM(K) = WP(K)/AM(K)                                       P1712   02064
      IF(RHO(K).NE.0.)RHO(K)=WP(K)/RHO(K)                       P1712   02065
      DO 215 J=1,L                                              P1712   02066
      BOP(J,K)=BOP(J,K)/WP(K)                                   P1712   02067
      IF(V(J).LT.0.)VMIN(K)= VMIN(K)+BOP(J,K)*V(J)              P1712   02068
      IF(V(J).GT.0.)VPLS(K)=VPLS(K)+BOP(J,K)*V(J)               P1712   02069
  215 CONTINUE                                                  P1712   02070
      IF(MOLES) GO TO 220                                       P1712   02071
      DO 218 N=1,NREAC                                          P1712   02072
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      IF(FOX(N).EQ.OX.AND.K.EQ.2)  GO TO 218          P1712  02073
      IF(FOX(N).NE.OX.AND.K.EQ.1)  GO TO 218          P1712  02074
      PECWT(N) = PECWT(N)/WP(K)                       P1712  02075
                                                      P1712  02076
  218 CONTINUE                                        P1712  02077
  220 CONTINUE                                        P1712  02078
      NEWR=.TRUE.                                     P1712  02079
      DO 230 N = 1,NREAC                              P1712  02080
      IF (DENS(N).NE.C.) GO TO 230                    P1712  02081
      RHO (1) = 0.                                    P1712  02082
      GO TO 1000                                      P1712  02083
  230 CONTINUE                                        P1712  02084
 1000 RETURN                                          P1712  02085
      END
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      SUBROUTINE RKTOUT                                                P1712  02086
C                                                                      P1712  02087
C     ROCKET PERFORMANCE PERAMETERS                                    P1712  02088
C                                                                      P1712  02089
C                                                                      P1712  02090
      LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,SHOCK                       P1712  02091
C                                                                      P1712  02092
      DIMENSION NV(13),Z(10,4)                                         P1712  02093
      DIMENSION VELOC(13)                                              P1712  02094
C                                                                      P1712  02095
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)      P1712  02096
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) P1712  02097
     2 ,TOTN(13)                                                       P1712  02098
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)  P1712  02099
     1 ,DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)            P1712  02100
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2) P1712  02101
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  02102
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        P1712  02103
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  02104
     4 ,RHOP,RMW(15),TLN,JANF                                          P1712  02105
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  02106
     1  FMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ    P1712  02107
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                  P1712  02108
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  02109
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                            P1712  02110
      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)    P1712  02111
     1  ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2        P1712  02112
     2  ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,F0                       P1712  02113
      COMMON/CVOLUM/ VOLUMC,IMPETUS,IFLGGG                             P1712  02114
      REAL IMPETUS                                                     P1712  02115
C                                                                      P1712  02116
      EQUIVALENCE (V,NV),(Z,H0)                                        P1712  02117
C                                                                      P1712  02118
      DATA EXIT/4HEXIT/                                                P1712  02119
C                                                                      P1712  02120
      IF(EQL) WRITE (6,37)                                             P1712  02121
   37 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING E P171201 00007
     1QUILIBRIUM COMPOSITION DURING EXPANSION        *//)              P1712  02123
      IF (.NOT.EQL) WRITE (6,38)                                       P1712  02124
   38 FORMAT(1H1/20X,* THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING F P171201 00008
     1ROZEN COMPOSITION DURING EXPANSION        *//)                   P1712  02126
      IF (TPSP) WRITE (6,737)                                          P1712  02127
  737 FORMAT (52X,28HAT AN ASSIGNED TEMPERATURE          )             P1712  02128
      V(1) = PPP(1)*14.696006                                          P1712  02129
      WRITE (6,40) V(1)                                                P1712  02130
   40 FORMAT(5H PC = ,F8.1,5H PSIA)                                    P1712  02131
      CALL OUT1                                                        P1712  02132
      NEX = NPT - 2                                                    P1712  02133
      DO 862 I = 1,NEX                                                 P1712  02134
  862 V(I) = EXIT                                                      P1712  02135
      WRITE(6,48) (V(I),I=1,NEX)                                       P1712  02136
   48 FORMAT(1H0,16X,16HCHAMBER   THROAT  ,11(5X,A4))                  P1712  02137
C                                                                      P1712  02138
```

```
C     PRESSURE RATIOS                                                   P1712  02139
C                                                                       P1712  02140
      DO 45 I=1,NPT                                                     P1712  02141
      K= 2*I+3                                                          P1712  02142
      FMT(K)= F3                                                        P1712  02143
      IF (PCP(I).GE.1000.) FMT(K)=F2                                    P1712  02144
      IF (PCP(I).GE.10000.)FMT(K)=F1                                    P1712  02145
      IF (PCP(I).GE.1300000.)FMT(K) = F0                                P1712  02146
   45 CONTINUE                                                          P1712  02147
      WRITE (6,FMT) FR1,FB,FB,FB,(PCP(J),J=1,NPT)                       P1712  02148
      CALL OUT2                                                         P1712  02149
C                                                                       P1712  02150
      AGV = 9.80665                                                     P1712  02151
      DO 202 K=2,NPT                                                    P1712  02152
      SPIM(K) = (2.*RR*(HSUM(1)-HSUM(K)))**.5/AGV                       P1712  02153
C                                                                       P1712  02154
C  AW (A/W) IN UNITS OF SEC/ATM                                         P1712  02155
C                                                                       P1712  02156
      AW = RR*TTT(K)/(PPP(K)*          WM(K)*SPIM(K)*AGV**2)            P1712  02157
      IF(K.NE.2)GO TO 200                                               P1712  02158
      AWT=AW                                                            P1712  02159
      CSTR=32.174*P(1)*AWT                                              P1712  02160
  200 AEAT(K)=AW/AWT                                                    P1712  02161
      VACI(K)=SPIM(K)+PPP(K)*AW                                         P1712  02162
      IF (SONVEL(K).NE.0.) VMOC(K)=SPIM(K)*AGV/SONVEL(K)                P1712  02163
      NV(K)= CSTR + .5                                                  P1712  02164
  202 CONTINUE                                                          P1712  02165
C                                                                       P1712  02166
C   MACH NUMBER                                                         P1712  02167
C                                                                       P1712  02168
      VMOC(1)=0.                                                        P1712  02169
      IF(GAMMAS(2).EQ.0.) VMOC(2)=0.                                    P1712  02170
      FMT(7) = F3                                                       P1712  02171
      WRITE(6,FMT)(FN(I),I=1,4),(VMOC(J),J=1,NPT)                       P1712  02172
C                                                                       P1712  02173
C  VELOCITY                                                             P1712  02174
C                                                                       P1712  02175
      DO 1202 I=1,NPT                                                   P1712  02176
      VELOC(I)=SONVEL(I)*VMOC(I)*3.280840                               P1712  02177
 1202 CONTINUE                                                          P1712  02178
      WRITE(6,1203)(VELOC(I),I=1,NPT)                                   P1712  02179
 1203 FORMAT(1H ,*VEL, FT/SEC    *,13F9.1)                              P1712  02180
      CALL VISCON(NS,NPT,SUB,EN,TOTN,TTT)                               P171201 00009
      IF(IFLGGG.GT.0) GO TO 203                                         P1712  02181
C                                                                       P1712  02182
C  CONSTANT VOLUME AND IMPETUS                                          P1712  02183
C                                                                       P1712  02184
      IVOLUMC=VOLUMC+.5                                                 P1712  02185
      WRITE(6,9000) IVOLUMC,IMPETUS                                     P1712  02186
 9000 FORMAT(1H ,*T, CV, DEG K*,6X,I5/1H ,*IMPETUS        *,F7.0)       P1712  02187
  203 WRITE(6,208)                                                      P1712  02188
  208 FORMAT (1H )                                                      P1712  02189
C                                                                       P1712  02190
```

```
C     C
C
      FMT(4) = FMT9X
      FMT(5) = FMT13
      FMT(6) = FMTI9
      FMT(7) = F8
      WRITE(6,FMT)(FR(I),I=1,4),(NV(J),J=2,NPT)
C
C     CF - THRUST COEFICIENT
C
      FMT(6) = FMT(8)
      FMT(7) = F3
      DO 212  I=2,NPT
  212 V(I)=32.174*SPIM(I)/CSTR
      WRITE(5,FMT)FC1,F8,F8,F8,(V(J),J=2,NPT)
C
C     AREA RATIO
C
      FMT(5) = F8
      DO 214 I = 2,NPT
      K = 2*I+3
      FMT(K) = F4
      IF (AEAT(I).GE.1.) FMT(K) = F3
      IF (AEAT(I).GE.10.) FMT(K) = F2
      IF (AEAT(I).GE.100.) FMT(K) = F1
  214 CONTINUE
      WRITE(6,FMT)FA1,FA2,F8,F8,(AEAT(J),J=2,NPT)
C
C     VACUUM IMPULSE
C
      FMT(5) = FMT13
      FMT(7) = F1
      WRITE(6,FMT)(FA(I),I=1,4),(VASI(J),J=2,NPT)
C
C     SPECIFIC IMPULSE
C
      WRITE(6,FMT)(FI(I),I=1,4),(SPIM(J),J=2,NPT)
      WRITE (6,208)
      FMT(4) = F8
      FMT(5) = FMT13
      FMT(7) = F5
      IF(EQL)  GO TO 312
      WRITE(6,310)
  310 FORMAT(15HMOLE FRACTIONS //)
C
C     MOLE FRACTIONS - FROZEN
C
      LINE = 0
      DO 430 K =1,NS
      V(LINE+1) = EN(K,1)/TOTN(1)
      IF (V(LINE+1).LT.(5.E-6))  GO TO 424
      LINE = LINE+1
      Z(LINE,1) = SUB(K,1)
```

```
      Z(LINE,2) = SUB(K,2)                                          P1712  02244
      Z(LINE,3) = SUB(K,3)                                          P1712  02245
      Z(LINE,4) = V(LINE)                                           P1712  02246
  424 IF (LINE.NE.4.AND.K.NE.NS)  GO TO 430                         P1712  02247
      IF (LINE.EQ.0)  GO TO 312                                     P1712  02248
      WRITE (6,426) (Z(LN,1),Z(LN,2),Z(LN,3),Z(LN,4),LN=1,LINE)     P1712  02249
  426 FORMAT (1H ,4(3A4,F9.5,7X))                                   P1712  02250
      LINE = 0                                                      P1712  02251
  430 CONTINUE                                                      P1712  02252
  312 CALL OUT3                                                     P1712  02253
 1000 RETURN                                                        P1712  02254
      END                                                           P1712  02255
```

```
      SUBROUTINE ROCKET                                                 P1712  02256
C                                                                       P1712  02257
C                                                                       P1712  02258
C     ROCKET PERFORMANCE                                                P1712  02259
C     EITHER HPSP OR TPSP IS TRUE                                       P1712  02260
C                                                                       P1712  02261
      LOGICAL HP,SP,TP,IDEBUG,NEWR ,IONS,MOLES,FROZ,EQL,LOGV,HPSP,TPSP   P1712  02262
C                                                                       P1712  02263
      DIMENSION AA(2),BB(2),CC(2)                                       P1712  02264
C                                                                       P1712  02265
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)       P1712  02266
     1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)  P1712  02267
     2,TCTN(13)                                                         P1712  02268
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  02269
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  02270
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2)  P1712  02271
     1 ,TN,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) P1712  02272
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  02273
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  02274
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  02275
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TSP,MOLES,NP,NT,NPT,L,NS, P1712  02276
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  02277
     2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  02278
      COMMON/PERF/PCP(26),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) P1712  02279
     1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO                             P1712  02280
      COMMON/CVOLUM/ VOLUMC,IMPETUS,IFLGGG                              P1712  02281
      REAL IMPETUS                                                      P1712  02282
C                                                                       P1712  02283
      NAMELIST/RKTINP/EQL,FROZ,SUBAR,SUPAR,PCP                          P1712  02284
C                                                                       P1712  02285
      ITN = 0                                                           P1712  02286
      IFLGGG=0                                                          P1712  02287
  210 DO 300 I=1,26                                                     P1712  02288
      PCP(I)= 0.                                                        P1712  02289
      SUBAR(I) = 0.                                                     P1712  02290
  300 CONTINUE                                                          P1712  02291
      HPSP = .TRUE.                                                     P1712  02292
      HP = .TRUE.                                                       P1712  02293
      TPSP = .FALSE.                                                    P1712  02294
      EQL = .TRUE.                                                      P1712  02295
      FROZ = .TRUE.                                                     P1712  02296
      READ (5,RKTINP)                                                   P1712  02297
      IF (T(1).EQ.0.)  GO TO 302                                        P1712  02298
      TPSP = .TRUE.                                                     P1712  02299
      TP = .TRUE.                                                       P1712  02300
      HPSP = .FALSE.                                                    P1712  02301
      GO TO 303                                                         P1712  02302
  302 T(1) = 3800.                                                      P1712  02303
  303 IF (PCP(1).NE.0.)  GO TO 306                                      P1712  02304
      DO 305  I=1,NP                                                    P1712  02305
      K = NP-I+2                                                        P1712  02306
      P(K) = P(K-1)                                                     P1712  02307
  305 CONTINUE                                                          P1712  02308
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      GO TO 311                                                          P1712 02309
  308 NP= 2                                                              P1712 02310
      DO 310 I=1,24                                                      P1712 02311
      IF (I.GT.2) GO TO 309                                              P1712 02312
      IF ((PCP(I).EQ.0.).OR.PCP(I).EQ.1.) GO TO 310                      P1712 02313
  309 IF (PCP(I).EQ.0.) GO TO 311                                        P1712 02314
      NP = NP + 1                                                        P1712 02315
      P(NP) = P(1)/PCP(I)                                                P1712 02316
  310 CONTINUE                                                           P1712 02317
  311 NSUB=0                                                             P1712 02318
      NSUP = 0                                                           P1712 02319
      DO 320  I=1,13                                                     P1712 02320
      IF(SUBAR(I).NE.0.)NSUB=NSUB+1                                      P1712 02321
      IF(SUPAR(I).NE.0.)NSUP=NSUP+1                                      P1712 02322
  320 CONTINUE                                                           P1712 02323
      WRITE (6,RKTINP)                                                   P1712 02324
      SS0 = 0.                                                           P1712 02325
      ITROT= 3                                                           P1712 02326
      TT = T(1)                                                          P1712 02327
C                                                                        P1712 02328
C     SET ASSIGNED P                                                     P1712 02329
C                                                                        P1712 02330
      DO 902 IP = 1,NP                                                   P1712 02331
      PP = P(IP)                                                         P1712 02332
      CALL EQLBRM                                                        P1712 02333
      T(NPT) = TT                                                        P1712 02334
      IF(TT.NE.0.)  GO TO 333                                            P1712 02335
      IF(NPT.EQ.0)  GO TO 1000                                           P1712 02336
      GO TO 900                                                          P1712 02337
  333 PCP(NPT) = P(1)/PP                                                 P1712 02338
      IF(IP.GT.1)  GO TO 195                                             P1712 02339
C                                                                        P1712 02340
C     COMBUSTION CHAMBER                                                 P1712 02341
C                                                                        P1712 02342
      TP = .FALSE.                                                       P1712 02343
      HP = .FALSE.                                                       P1712 02344
      SP = .TRUE.                                                        P1712 02345
      S0 = SSUM(1)                                                       P1712 02346
      PCP(2)=((GAMMAS(1)+1.)/2.)**(GAMMAS(1)/(GAMMAS(1)-1.))             P1712 02347
      P(2) = P(1)/PCP(2)                                                 P1712 02348
      TT = 2.*TT/(GAMMAS(1)+1.)                                          P1712 02349
      GO TO 900                                                          P1712 02350
  195 IF(IP.GT.2) GO TO 900                                              P1712 02351
C                                                                        P1712 02352
C     THROAT                                                             P1712 02353
C                                                                        P1712 02354
  190 IF(ITH.NE.2)  GO TO 191                                            P1712 02355
      ITH = 0                                                            P1712 02356
      GAMMAS(2) = 0.                                                     P1712 02357
      GO TO 900                                                          P1712 02358
  191 DH = HSUM(1)-HSUM(2)                                               P1712 02359
      DHSTAR = DH-GAMMAS(2)*TT*ENN/2.                                    P1712 02360
      IF (IDEBUG) WRITE(6,923)DHSTAR,HSUM(1),HSUM(2),PCP(2)              P1712 02361
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  923 FORMAT(4E25.8)                                              P1712 02362
      DH = DHSTAR/DH                                              P1712 02363
      IF(DH.LT.0.) DH=-DH                                         P1712 02364
      IF(DH.LE.0.4E-4.OR.ITROT.EQ.0)  GO TO 900                   P1712 02365
      IF(JSOL.NE.0) ITH =1                                        P1712 02366
      IF (JSOL.EQ.0.AND.ITH.EQ.1) ITH=2                           P1712 02367
      IF(ITH.EQ.0) GO TO 192                                      P1712 02368
C                                                                 P1712 02369
C     SPECIAL THROAT INTERPOLATION IF ITH = 2                     P1712 02370
C                                                                 P1712 02371
      DLNI = .5*TT*ENN/(HSUM(1)-HSUM(2))                          P1712 02372
      AA(ITH)=.5*DLNI*(2.*DLNI+(GAMMAS(2)-1.)/GAMMAS(2))          P1712 02373
      XX = ALOG(PCP(2))                                           P1712 02374
      BB(ITH) = 1./GAMMAS(2)-DLNI-2.*XX*AA(ITH)                   P1712 02375
      CC(ITH) = ENN*TT/(PP*(HSUM(1)-HSUM(2))**.5)                 P1712 02376
      CC(ITH) = ALOG(CC(ITH))-XX*(BB(ITH)+AA(ITH)*XX)             P1712 02377
      IF(ITH.EQ.1)  GO TO 192                                     P1712 02378
      BB(1)=BB(1)-BB(2)                                           P1712 02379
      AA(1)=AA(1)-AA(2)                                           P1712 02380
      PCP(2)=(-BB(1)+(BB(1)*BB(1)-4.*AA(1)*(CC(1)-CC(2)))**.5)/(2.*AA(1) P1712 02381
     1)                                                           P1712 02382
      PCP(2)=EXP(PCP(2))                                          P1712 02383
      GO TO 193                                                   P1712 02384
  192 PCP(2)= PCP(2)/(1.+2.*DHSTAR/(ENN*TT *(GAMMAS(2)+1.)))      P1712 02385
  193 P(2) = P(1) / PCP(2)                                        P1712 02386
      PP = P(2)                                                   P1712 02387
      ITROT = ITROT-1                                             P1712 02388
      CALL EQLBRM                                                 P1712 02389
      IF(TT.EQ.0.) GO TO 1000                                     P1712 02390
      GO TO 190                                                   P1712 02391
C                                                                 P1712 02392
  900 K = 0                                                       P1712 02393
      IF (.NOT.EQL .AND. FROZ) GO TO 990                          P1712 02394
      IF(IP.EQ.NP.OR.TT.EQ.0.)   GO TO 860                        P1712 02395
      K = NPT                                                     P1712 02396
      IF(NPT.NE.13)  GO TO 870                                    P1712 02397
  860 CALL RKTOUT                                                 P1712 02398
      IFLGGG=1                                                    P1712 02399
      IF ((NSUB + NSUP).NE.0) CALL RATIO                          P1712 02400
      IF(K.EQ.0) GO TO 990                                        P1712 02401
      WRITE(6,865)                                                P1712 02402
  865 FORMAT(1H1)                                                 P1712 02403
      NPT = 2                                                     P1712 02404
  870 NPT = NPT + 1                                               P1712 02405
C                                                                 P1712 02406
C   SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT                 P1712 02407
C                                                                 P1712 02408
      DO 880 I = 1,NS                                             P1712 02409
      EN(I,NPT) = EN(I,K)                                         P1712 02410
  880 CONTINUE                                                    P1712 02411
  902 CONTINUE                                                    P1712 02412
  990 IF (FROZ) CALL FROZEN                                       P1712 02413
 1000 RETURN                                                      P1712 02414
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160          END                                                   P1712   02415
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      SUBROUTINE SEARCH                                                 P1712  02416
C                                                                       P1712  02417
C  SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED             P1712  02418
      INTEGER SUB,OMIT,END                                              P1712  02419
C                                                                       P1712  02420
      LOGICAL NEWR                                                      P1712  02421
C                                                                       P1712  02422
      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3)                          P1712  02423
C                                                                       P1712  02424
      COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)   P1712  02425
     1 ,CELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)             P1712  02426
      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)  P1712  02427
     1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUBJ,AC(2),AM(2) P1712  02428
     2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)         P1712  02429
     3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) P1712  02430
     4 ,RHOP,RMW(15),TLN,JANF                                           P1712  02431
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  02432
     1  KMAT,IMAT,IQ1,N,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ     P1712  02433
     2 ,IONS,KC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                   P1712  02434
C                                                                       P1712  02435
      EQUIVALENCE (DATE,EN),(OMIT,ENLN),(ENDD,END)                      P1712  02436
C                                                                       P1712  02437
      DATA  GAS/1HG/,END/3HEND/                                         P1712  02438
C                                                                       P1712  02439
      NC= 0                                                             P1712  02440
      IX= 0                                                             P1712  02441
      COEF(1,1,1) = ENDD                                                P1712  02442
      DO 3 I=1,150                                                      P1712  02443
      ISAVE=I                                                           P1712  02444
      IF(A(1,I).EQ.ENDD)  GO TO 4                                       P1712  02445
      DO 3  J=1,L                                                       P1712  02446
      A(J,I) = 0.                                                       P1712  02447
    3 CONTINUE                                                          P1712  02448
    4 MAXNS=ISAVE                                                       P1712  02449
      REWIND 9                                                          P1712  02450
      READ (9,5) TLOW,TMID,THIGH                                        P1712  02451
    5 FORMAT (3F10.3)                                                   P1712  02452
      NS = 1                                                            P1712  02453
    7 READ    (9,10)(SUB(NS,I),I=1,3),DATE(1,NS),DATE(2,NS),(MT(J),B(J), P1712  02454
     1  J=1,4),PHAZ,T1,T2                                               P1712  02455
   10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3)                           P1712  02456
      IF(SUB(NS,1).EQ.END) GO TO 171                                    P1712  02457
      READ (9,20)((COEF(I,J,NS),J=1,7),I=1,2)                           P1712  02458
   20 FORMAT (5E15.8)                                                   P1712  02459
      IF(NOMIT.EQ.0) GO TO 810                                          P1712  02460
      DO 805 I=1,NOMIT                                                  P1712  02461
      DO 804 J=1,3                                                      P1712  02462
      IF(OMIT(J,I).NE.SUB(NS,J)) GO TO 805                              P1712  02463
  804 CONTINUE                                                          P1712  02464
      GO TO 7                                                           P1712  02465
  805 CONTINUE                                                          P1712  02466
  810 DO 820 K=1,4                                                      P1712  02467
      IF(B(K).EQ.0.) GO TO 825                                          P1712  02468
```

```
          DO 168 I=1,L                                              P1712  02469
          IF(LLMT(I).EQ.MT(K)) GO TO 820                            P1712  02470
      168 CONTINUE                                                  P1712  02471
          DO 819 J=1,L                                              P1712  02472
      819 A(J,NS) = 0.                                              P1712  02473
          GO TO 7                                                   P1712  02474
      820 A(I,NS)= B(K)                                             P1712  02475
      825 IF(NS.EQ.MAXNS)  GO TO 870                                P1712  02476
          IUSE(NS)= 0                                               P1712  02477
          IF(PHAZ.EQ.GAS) GO TO 170                                 P1712  02478
          NC= NC+1                                                  P1712  02479
          TEMP(NC,1)= T1                                            P1712  02480
          TEMP(NC,2)= T2                                            P1712  02481
          IX= IX+1                                                  P1712  02482
          IF(IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145                P1712  02483
          DO 830 I=1,L                                              P1712  02484
          IF(A(I,NS).NE.A(I,NS-1)) GO TO 145                        P1712  02485
      830 CONTINUE                                                  P1712  02486
          IX= IX-1                                                  P1712  02487
      145 IUSE(NS)= -IX                                             P1712  02488
      170 NS= NS+1                                                  P1712  02489
          GO TO 7                                                   P1712  02490
      870 WRITE(6,871) (SUB(NS,J),J=1,3)                            P1712  02491
      871 FORMAT (45H0DIMENSIONS IN/SPECES/TOO SMALL TO CONSIDER ,3A4)  P1712  02492
          GO TO 7                                                   P1712  02493
      171 NS= NS-1                                                  P1712  02494
          NEWR= .FALSE.                                             P1712  02495
          WRITE(6,172)                                              P1712  02496
      172 FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM   )    P1712  02497
          DO 174 I=1,NS,5                                           P1712  02498
          I5= I+4                                                   P1712  02499
          IF(NS.LT.I5) I5=NS                                        P1712  02500
      174 WRITE (6,176)(DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I,  P1712  02501
         1  I5)                                                     P1712  02502
      176 FORMAT(5(5X,2A3,2X,3A4))                                  P1712  02503
          RETURN                                                    P1712  02504
          END                                                       P1712  02505
```

```
      SUBROUTINE SET(ONE,TWO,THREE,ARG,HAL)                              P1712  02506
C                                                                        P1712  02507
C     (USED FOR AREA RATIO INTERPOLATION ONLY)                           P1712  02508
C     SETS UP ALL 4 BY 5 MATRICES                                        P1712  02509
C                                                                        P1712  02510
C     DOUBLE PRECISION A,ANS,G,X                                         P1712  02511
C                                                                        P1712  02512
      DIMENSION ANS(6),ONE(2),TWO(2),THREE(2),A(20,21)                   P1712  02513
C                                                                        P1712  02514
      COMMON/DOUBLE/G(20,21),X(20)                                       P1712  02515
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS, P1712  02516
     1  KMAT,IMAT,IG1,N,J,NOMIT,IF,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ      P1712  02517
     2 ,IONS,NO,NSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2                    P1712  02518
C                                                                        P1712  02519
      EQUIVALENCE (G,A),(X,ANS)                                          P1712  02520
C                                                                        P1712  02521
      DO 8 J=1,2                                                         P1712  02522
      A(J,5)=ALOG(ONE(J))                                                P1712  02523
      A(J+2,5)=TWO(J)                                                    P1712  02524
      A(J,2)=ALOG(THREE(J))                                              P1712  02525
    8 CONTINUE                                                           P1712  02526
      DO 1 I=1,2                                                         P1712  02527
      A(I,1)=1.0                                                         P1712  02528
      A(I+2,1)=0.0                                                       P1712  02529
      A(I+2,2)=1.0                                                       P1712  02530
      DO 1 J=2,3                                                         P1712  02531
      A(I,J+1)=A(I,2)**J                                                 P1712  02532
      MXP=J-1                                                            P1712  02533
      A(I+2,J+1)=A(I,2)**MXP*FLOAT(J)                                    P1712  02534
    1 CONTINUE                                                           P1712  02535
      IMAT = 4                                                           P1712  02536
      CALL MGAUSD                                                        P1712  02537
      HAL=ANS(1)                                                         P1712  02538
      SUM=ALOG(ARG)                                                      P1712  02539
      DO 10 J=1,3                                                        P1712  02540
      HAL=HAL+SUM**J*(ANS(J+1))                                          P1712  02541
   10 CONTINUE                                                           P1712  02542
      HAL=EXP(HAL)                                                       P1712  02543
      RETURN                                                             P1712  02544
      END                                                                P1712  02545
```

SUBROUTINE VISCON FORTRAN EXTENDED VERSION 2.0 31/12/70 C .09.56. PAGE NO. 1

```
      SUBROUTINE VISCON(NS,NPT,SUB,EN,TOTN,T)                          P171201 00010
C                                                                       P171201 00011
C   THIS SUBROUTINE COMPUTES THE VISCOSITY AND THE CONDUCTIVITY         P171201 00012
C   OF A GAS MIXTURE CONSISTING OF 5 GASEOUS SPECIES.                   P171201 00013
C   GASEOUS SPECIES TO BE CONSIDERED ARE H2O,CO,H2,CO2,AND N2.          P171201 00014
C                                                                       P171201 00015
      COMMON/PRCENT/ FMOLE                                              P171201 00016
      DIMENSION SUB(150,3),EN(150,13),TOTN(13),T(13),SPECE(5),EK(5),    P171201 00017
     1SIG(5),WGTM(5),TE(33),OMEG(33),FMOLE(5),VIS(5),COND(5),           P171201 00018
     2VISMIX(13),CONMIX(13)                                             P171201 00019
      DATA (SPECE(I),I=1,5)/4HH2O ,4HCO  ,4HH2  ,4HCO2 ,4HN2  /         P171201 00020
      DATA (SIG(I),I=1,5)/2.824,3.706,2.915,3.897,3.749/                P171201 00021
      DATA (EK(I),I=1,5)/230.9,89.0,38.0,213.0,79.8/                    P171201 00022
      DATA (WGTM(I),I=1,5)/18.,28.01,2.016,44.01,28.02/                 P171201 00023
      DATA CON1,CON2,CONS/ 0.000026693,0.00019891,0.35355339059/        P171201 00024
      DATA (TE(I),I=1,33)/1.0,1.2,1.4,1.6,1.8,2.0,2.2,2.4,2.6,2.8,3.0,  P171201 00025
     13.2,3.4,3.6,3.8,4.0,5.0,6.0,7.0,8.0,9.0,10.0,11.0,12.0,13.0,14.0, P171201 00026
     215.0,16.0,32.0,64.0,128.0,256.0,512.0/                            P171201 00027
      DATA (OMEG(I),I=1,33)/1.5938,1.4568,1.3557,1.2900,1.2216,1.1791,  P171201 00028
     11.1377,1.1066,1.0803,1.0579,1.0385,1.0214,1.0063,0.9928,0.9807,   P171201 00029
     20.9696,0.9265,0.8960,0.8725,0.8536,0.8378,0.8242,0.8123,0.8017,   P171201 00030
     30.7922,0.7836,0.7756,0.7883,0.6939,0.6262,0.5634,0.5056,0.4528/   P171201 00031
C                                                                       P171201 00032
C   VALUES FOR VISCOSITY AND CONDUCTIVITY WILL BE COMPUTED AT THE       P171201 00033
C   CHAMBER,THE THROAT,AND AT THE ASSIGNED EXITS.                       P171201 00034
C                                                                       P171201 00035
C      WRITE(6,8999) NS,NPT                                             P171201 00036
 8999 FORMAT(2I10)                                                      P171201 00037
      PMOLE=0.0                                                         P171201 00038
         DO 1000 M=1,NPT                                                P171201 00039
C                                                                       P171201 00040
C   COMPUTE THE MOLE FRACTIONS OF THE 5 GASEOUS SPECIES.                P171201 00041
C                                                                       P171201 00042
      DO 20 I=1,5                                                       P171201 00043
      DO 10 J=1,NS                                                      P171201 00044
C                                                                       P171201 00045
C   SEARCH THE ARRAY SUB(J,1) FOR THE 5 NEEDED SPECIES. WHEN ONE OF THE P171201 00046
C   NEEDED SPECIES IS FOUND,COMPUTE THE MOLE FRACTION.                  P171201 00047
C                                                                       P171201 00048
      IF(SPECE(I).NE.SUB(J,1)) GO TO 10                                 P171201 00049
      FMOLE(I)=EN(J,M)/TOTN(M)                                          P171201 00050
C     WRITE(6,9000) SPECE(I),SUB(J,1),EN(J,M),TOTN(M),FMOLE(I),I,J,M    P171201 00051
 9000 FORMAT(1X,2A10,3F15.8,3I5)                                        P171201 00052
      IF(M.EQ.1) PMOLE=PMOLE+FMOLE(I)*100.                              P171201 00053
      GO TO 20                                                          P171201 00054
   10 CONTINUE                                                          P171201 00055
C   IF THE SPECIE CANNOT BE LOCATED IN THE ARRAY SUB(J,1), SET THE MOLE P171201 00056
C   FRACTION TO MINUS ONE.                                              P171201 00057
C                                                                       P171201 00058
      FMOLE(I)=-1.0                                                     P171201 00059
   20 CONTINUE                                                          P171201 00060
C                                                                       P171201 00061
C   COMPUTE THE VISCOSITY AND THE CONDUCTIVITY FOR EACH OF THE 5 SPECIES P171201 00062
```

```
      C                                                                    P171201 00063
            DO 100 I=1,5                                                   P171201 00064
            IF(FMOLE(I).LT.0.0) GO TO 100                                  P171201 00065
            TEK=T(M)/EK(I)                                                 P171201 00066
            IF(TEK.LT.TE(1)) TEK=TE(1)                                     P171201 00067
            IF(TEK.GT.TE(33)) TEK=TE(33)                                   P171201 00068
            DO 40 J=1,33                                                   P171201 00069
            IF(TEK-TE(J)) 30,25,40                                         P171201 00070
         25 DCM=OMEG(J)                                                    P171201 00071
            GO TO 50                                                       P171201 00072
         30 FRAC=(TEK-TE(J-1))/(TE(J-1)-TE(J))                             P171201 00073
            DOM=OMEG(J-1)+FRAC*(OMEG(J-1)-OMEG(J))                         P171201 00074
            GO TO 50                                                       P171201 00075
         40 CONTINUE                                                       P171201 00076
         50 DIV=SIG(I)*SIG(I)*DOM                                          P171201 00077
      C                                                                    P171201 00078
      C   VISCOSITY                                                        P171201 00079
      C                                                                    P171201 00080
            VIS(I)=CONI*SQRT(WGTM(I)*T(M))/DIV                             P171201 00081
      C                                                                    P171201 00082
      C   CONDUCTIVITY                                                     P171201 00083
      C                                                                    P171201 00084
            COND(I)=CON2*SQRT(T(M)/WGTM(I))/DIV                            P171201 00085
      C     WRITE(6,9001) T(M),EK(I),TEK,TE(J-1),TE(J),FRAC,OMEG(J-1),OMEG(J), P171201 00086
      C    1DIV,DOM,SIG(I),WGTM(I),VIS(I),COND(I),I,J,M                    P171201 00087
       9001 FORMAT(8F15.8,/6F15.8,3I5)                                     P171201 00088
        100 CONTINUE                                                       P171201 00089
      C                                                                    P171201 00090
      C   COMPUTE VISCOSITY AND CONDUCTIVITY OF MIXTURE.                   P171201 00091
      C                                                                    P171201 00092
            VISMIX(M)=0.0                                                  P171201 00093
            CONMIX(M)=0.0                                                  P171201 00094
            DO 200 I=1,5                                                   P171201 00095
            SUM=0.0                                                        P171201 00096
            IF(FMOLE(I).LT.0.0) GO TO 200                                  P171201 00097
            DO 150 J=1,5                                                   P171201 00098
            IF(FMOLE(J).LT.0.0) GO TO 150                                  P171201 00099
            F1=SQRT(1.+WGTM(I)/WGTM(J))                                    P171201 00100
            F2=SQRT(VIS(I)/VIS(J))                                         P171201 00101
            F3=(WGTM(J)/WGTM(I))**(0.25)                                   P171201 00102
            FA=1.+F2*F3                                                    P171201 00103
            FAC=CONS/F1                                                    P171201 00104
            PHI=FAC*FA*FA                                                  P171201 00105
            SUM=SUM+FMOLE(J)*PHI                                           P171201 00106
      C     WRITE(6,9002) FMOLE(I),FMOLE(J),WGTM(I),WGTM(J),F1,VIS(I),VIS(J), P171201 00107
      C    1F2,COND(I),COND(J),F3,FA,FAC,PHI,SUM,I,J,M                     P171201 00108
       9002 FORMAT(8F15.8/7F15.8,3I5)                                      P171201 00109
        150 CONTINUE                                                       P171201 00110
      C                                                                    P171201 00111
      C   VISCOSITY OF MIXTURE                                             P171201 00112
      C                                                                    P171201 00113
            VISMIX(M)=VISMIX(M)+FMOLE(I)*VIS(I)/SUM                        P171201 00114
      C                                                                    P171201 00115
```

```
C     CONDUCTIVITY OF MIXTURE                                     P171201 00116
C                                                                 P171201 00117
      CONMIX(M)=CONMIX(M)+FMOLE(I)*COND(I)/SUM                    P171201 00118
C     WRITE(6,9009) VISMIX(M),CONMIX(M),M                         P171201 00119
 9009 FORMAT(1X,2F15.11,3X,I5)                                    P171201 00120
  200 CONTINUE                                                    P171201 00121
 1000 CONTINUE                                                    P171201 00122
      WRITE(6,2000) (VISMIX(I),I=1,NPT)                           P171201 00123
      WRITE(6,2100) (CONMIX(I),I=1,NPT)                           P171201 00124
 2000 FORMAT(1H ,*VISC, G/CM-SEC*,13F9.6)                         P171201 00125
 2100 FORMAT(1H ,*C, CAL/G-SEC-K*,13F9.6)                         P171201 00126
      RETURN                                                      P171201 00127
      END                                                         P171201 00128
```

APPENDIX II

POLYNOMIAL FIT PROGRAM

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```
      PROGRAM SLSQF(INPUT,OUTPUT)
      DIMENSION TT(100),CPR(100),HTR(100),STR(100)
      DIMENSION CCPR(100),CHTR(100),CSTR(100)
      DIMENSION NPT(2),NAME(6)
      COMMON/MATRIX/ G(10,11),X(10),IMAT
      R=1.98726
      ASSIGN 500 TO MEOF
      IF(EOF(MEOF)) 500,500,1
    1 READ 40,HO,NPT,NAME
   40 FORMAT(F10.1,2I3,4X,6A10)
      PRINT 112,NAME,HO
  112 FORMAT(1H1,29X,6A10//1P,5HHO = ,F10.1//)
      KPT=0
  111 KPT=KPT+1
      NVAL=NPT(KPT)
      READ 6,(TT(K),K=1,NVAL)
      READ 7,(CPR(K),K=1,NVAL)
      READ 7,(HTR(K),K=1,NVAL)
      DO 22 I=1,NVAL
   22 HTR(I)=HTR(I)*1000.+HO
      READ 7,(STR(K),K=1,NVAL)
    6 FORMAT(20F4.0)
    7 FORMAT(10F8.3)
      DO 16 I=1,10
      DO 15 J=1,11
      G(I,J)=0.
   15 CONTINUE
   16 CONTINUE
      SUMT=0.
      SUMT2=0.
      SUMT3=0.
      SUMT4=0.
      SUMT5=0.
      SUMT6=0.
      SUMT7=0.
      SUMT8=0.
      SUMTM2=0.
      DO 100 K=1,NVAL
      T=TT(K)
      CP=CPR(K)/R
      HT=HTR(K)/(R*T)
      ST=STR(K)/R
      TLOG=ALOG(T)
      T2=T**2
      T3=T2*T
      T4=T3*T
      T5=T4*T
      T6=T5*T
      T7=T6*T
      T8=T7*T
      TREC=1.0/T
      TM2=1.0/T2
      SUMT=SUMT+T
```

```
      SUMT2=SUMT2+T2
      SUMT3=SUMT3+T3
      SUMT4=SUMT4+T4
      SUMT5=SUMT5+T5
      SUMT6=SUMT6+T6
      SUMT7=SUMT7+T7
      SUMT8=SUMT8+T8
      SUMTM2=SUMTM2+TM2
      G(1,1)=G(1,1)+2.+TLOG**2
      G(1,2)=G(1,2)+(1.5+TLOG)*T
      G(1,3)=G(1,3)+(4./3.+.5*TLOG)*T2
      G(1,4)=G(1,4)+(1.25+TLOG/3.)*T3
      G(1,5)=G(1,5)+(1.2+TLOG/4.)*T4
      G(1,6)=G(1,6)+TREC
      G(1,7)=G(1,7)+TLOG
      G(1,11)=G(1,11)+CP+HT+ST*TLOG
      G(2,11)=G(2,11)+(CP+.5*HT+ST)*T
      G(3,11)=G(3,11)+(CP+HT/3.+.5*ST)*T2
      G(4,11)=G(4,11)+(CP+HT/4.+ST/3.)*T3
      G(5,11)=G(5,11)+(CP+HT/5.+ST/4.)*T4
      G(6,11)=G(6,11)+HT*TREC
      G(7,11)=G(7,11)+ST
      IF(K.GT.1) GO TO 50
      G(1,8)=1.0
      G(1,9)=1.0
      G(1,10)=TLOG
      G(2,6)=FLOAT(NVAL)/2.0
      G(2,8)=T
      G(2,9)=T/2.0
      G(2,10)=T
      G(3,8)=T2
      G(3,9)=T2/3.
      G(3,10)=T2/2.
      G(4,8)=T3
      G(4,9)=T3/4.
      G(4,10)=T3/3.
      G(5,8)=T4
      G(5,9)=T4/5.
      G(5,10)=T4/4.
      G(6,9)=TREC
      G(7,7)=FLOAT(NVAL)
      G(7,10)=1.0
      G(8,11)=CP
      G(9,11)=HT
      G(10,11)=ST
   50 CONTINUE
  100 CONTINUE
      G(2,2)=(9./4.)*SUMT2
      G(2,3)=(5./3.)*SUMT3
      G(2,4)=(35./24.)*SUMT4
      G(2,5)=(27./20.)*SUMT5
      G(2,7)=SUMT
      G(3,3)=(49./36.)*SUMT4
```

```
      G(3,4)=(5./4.)*SUMT5
      G(3,5)=(143./120.)*SUMT6
      G(3,6)=SUMT/3.
      G(3,7)=SUMT2/2.
      G(4,4)=(169./144.)*SUMT6
      G(4,5)=(17./15.)*SUMT7
      G(4,6)=SUMT2/4.
      G(4,7)=SUMT3/3.
      G(5,5)=(441./400.)*SUMT8
      G(5,6)=SUMT3/5.
      G(5,7)=SUMT4/4.
      G(6,6)=SUMTM2
      DO 200 I=1,10
      DO 210 J=I,10
      IF(I.EQ.J) GO TO 210
      G(J,I)=G(I,J)
  210 CONTINUE
  200 CONTINUE
      PRINT 92
      IF(DEBUG(1).NE.0.0) GO TO 190
   92 FORMAT(1H ,*VALUES OF G*)
      DO 90 I=1,10
      PRINT 91,(G(I,J),J=1,11)
   91 FORMAT(1X,11E11.5)
   90 CONTINUE
  190 IMAT=10
      CALL MGAUSD
      PRINT 94
   94 FORMAT(1H ,*COEFFICIENTS ARE*)
      PRINT 192,X
  192 FORMAT(1X,7E15.8/1X,3E15.8)
      DO 400 I=1,NVAL
      T=TT(I)
      T2=T*T
      T3=T2*T
      T4=T3*T
      TLOG=ALOG(T)
      CCPR(I)=X(1)+X(2)*T+X(3)*T2+X(4)*T3+X(5)*T4
      CCPR(I)=CCPR(I)*R
      CHTR(I)=((X(1)+X(2)*T/2.+X(3)*T2/3.+X(4)*T3/4.+X(5)*T4/5.)*T+X(6))
     1*R
      CHTR(I)=(CHTR(I)-HO)/1000.
       CSTR(I)=(X(1)*TLOG+X(2)*T+X(3)*T2/2.+X(4)*T3/3.+X(5)*T4/4.+X(7)
     1R
  400 CONTINUE
      PRINT 401
  401 FORMAT(1H ,*   T         CP       CCP        HT       CHT        T       CST
     1    DCP     DHT      DST*//)
      DO 410 I=1,NVAL
      DCPR=ABS(CPR(I)-CCPR(I))
      DTR=(HTR(I)-HO)/1000.
      DHTS=ABS(DTR-CHTR(I))
      DSTR=ABS(STR(I)-CSTR(I))
```

```
  411 FORMAT(1H ,1X,F5.0,9F8.3)
      PRINT 411,TT(I),CPR(I),CCPR(I),DTR,CHTR(I),STR(I),CSTR(I),DCPR,
     1CHTR,DSTR
  410 CONTINUE
      GO TO (111,1),KPT
  500 CONTINUE
      END
```

```
                SUBROUTINE MGAUSD
          C
          C     SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS
          C
          C     DOUBLE PRECISION G,X,COEFX(20),SUM,Z
                DIMENSION COEFX(20)
          C
                COMMON/MATRIX/ G(10,11),X(10),IMAT
          C
                EQUIVALENCE (IUSE,IMAT)
          C
          C     DATA BIGNO/1.E+38/
                DATA BIGNO/1.E+320/
          C
          C     BEGIN ELIMINATION OF NNTH VARIABLE
          C
                IUSE1=IUSE+1
              6 DC 45 NN=1,IUSE
                IF (NN-IUSE) 8,83,8
             83 IF(G(NN,NN))31,23,31
          C
          C     SEARCH FO  AXIMUM COEFFICIENT IN EACH ROW
          C
              8 DC 18 I=NN,IUSE
                CCEFX(I) = BIGNO
                IF(G(I,NN).EQ.0.)  GO TO 18
                CCEFX(I) = 0.
                DC 10 J=NN,IUSE1
                SUM = G(I,J)
                IF(SUM.LT.0.)  SUM=-SUM
                IF(J.NE.NN)  GO TO 9
                Z = SUM
                GO TO 10
              9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM
             10 CCNTINUE
                COEFX(I) = COEFX(I)/Z
             18 CONTINUE
                TEMP = BIGNC
                I=0
             20 DO 22 J=NN,IUSE
                IF (COEFX(J)-TEMP) 87,22,22
             87 TEMP=COEFX(J)
                I=J
             22 CCNTINUE
                IF(I) 28,23,28
          C
          C     INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH
          C     VARIABLE FROM THE REMAINING EQUATIONS
          C
          C      INTERCHANGE EQUATIONS I AND NN
          C
             28 IF(NN-1) 29,31,29
             29 DO 30 J=NN,IUSE1
```

```
            Z=G(I,J)
            G(I,J)=G(NN,J)
            G(NN,J)=Z
         30 CONTINUE
      C
      C     DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH
      C     VARIABLE FROM THE REMAINING EQUATIONS
      C
         31 K = NN + 1
            DO 36 J = K, IUSE1
            IF((NN,NN).EQ.0.)  GO TO 23
                G(NN,J) = G(NN,J) / G(NN,NN)
         36 CONTINUE
            IF(K-IUSE1) 88,45,88
         88 DC 44 I = K,IUSE
         40 DO 44 J = K, IUSE1
                G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
         44 CONTINUE
         45 CONTINUE
      C
      C     BACKSOLVE FOR THE VARIABLES
      C
            K = IUSE
         47 J = K + 1
      C     X(K) = 0.0D0
            X(K) = 0.0
            SUM = 0.0
            IF(IUSE - J) 51,48,46
         48 DC 50 I = J,IUSE
                SUM = SUM + G(K,I)* X(I)
         50 CONTINUE
         51 X(K) = G(K,IUSE1) - SUM
            K = K - 1
            IF (K) 47,151,47
         23 IUSE = IUSE-1
        151 RETURN
            END
```

REFERENCES

1) Zeleznik, F. J, and Gordon, S. A General IBM 704 or 7090 Computer Program for Computation of Chemical Equilibrium Compositions, Rocket Performance, and Chapman-Jouget Detonations, NASA Technical Note TN D-1454, NASA Lewis Research Center, Cleveland, Ohio, October 1962. Unclassified.

2) Stull, D. R., et al. JANAF Thermochemical Tables, Dow Chemical Co., August 1965 (and Addenda).

3) Van Zeggern, F., and Storey, S. H. The Computation of Chemical Equilibria, Cambridge University Press, 1970.

4) Elements of Armament Engineering, Part I, Sources of Energy. AMCP 706-106, USAMC, August 1964.

5) Propellant Handbook, Technical Report AFRPL-TR-66-4 Rocket Propulsion Laboratory, Edwards Air Force Base, California, January 1966.

6) Hirschfelder, Curtiss, and Bird. Molecular Theory of Gases and Liquids, John Wiley, 1954.

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