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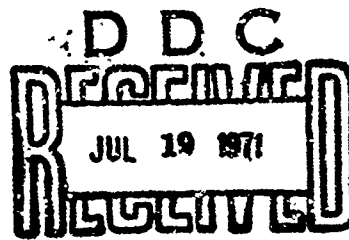
AD885781

**THEORETICAL GUN PROPELLANT
THERMOCHEMICAL EVALUATION**

**GUNS AND ROCKETS BRANCH
ADVANCED DEVELOPMENT DIVISION**

TECHNICAL REPORT AFATL-TR-71-11

JANUARY 1971



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Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) Advanced Development Division Air Force Armament Laboratory Eglin Air Force Base, Florida		2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED	
		2b. GROUP	
3. REPORT TITLE THEORETICAL GUN PROPELLANT THERMOCHEMICAL EVALUATION			
4. DESCRIPTIVE NOTES (Type of report and inclusive dates) Final Report - February 1970 to January 1971			
5. AUTHOR(S) (First name, middle initial, last name) Otto K. Heiney			
6. REPORT DATE January 1971		7a. TOTAL NO. OF PAGES 109	7b. NO. OF REFS 6
8a. CONTRACT OR GRANT NO. b. PROJECT NO 62602F 2560 c. d.		9a. ORIGINATOR'S REPORT NUMBER(S) AFATL -TR-71-11 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
10. DISTRIBUTION STATEMENT Distribution limited to U.S. Government agencies only; this report documents the test and evaluation of military hardware; limitation applied Jan 1971. Other requests for this document must be referred to the Air Force Armament Laboratory (DLDG), Eglin Air Force Base, Florida.			
11. SUPPLEMENTARY NOTES Available in DDC		12. SPONSORING MILITARY ACTIVITY Air Force Armament Laboratory Air Force Systems Command Eglin Air Force Base, Florida	
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.			

DD FORM 1473
1 NOV 63

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14	KEY WORDS	LINK A		LINK B		LINK C	
		ROLE	WT	ROLE	WT	ROLE	WT
	Gun Propellant Analysis NASA Lewis Algorithm Thermochemical Propellant Evaluation						

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Theoretical Gun Propellant Thermochemical Evaluation

Otto K. Heiney

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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

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

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 from 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:

$$dE + pdv - Tds < 0 \quad (1)$$

or at equilibrium

$$dE + pdv - Tds = 0 \quad (2)$$

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

$$d(E + pv - Ts) = 0 \quad (3)$$

$$G_T = H_T - T_1 S_1 \quad (4)$$

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 combustion species concentration and flame temperature (if the combustion pressure is specified). Then, to set up a minimization algorithm 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

$$H_T - H_{298} = \int_{298}^T C_p dT \quad (5)$$

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

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

$$\frac{C_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (7)$$

$$\frac{H_T}{RT} = a_1 + 1/2 a_2 T + 1/3 a_3 T^2 + 1/4 a_4 T^3 + 1/5 a_5 T^4 + a_6/T \quad (8)$$

$$\frac{S_T}{R} = a_1 \ln T + a_2 T + 1/2 a_3 T^2 + 1/3 a_4 T^3 + 1/4 a_5 T^4 + a_7 \quad (9)$$

For a more precise fit, the Lewis program utilizes two sets of coefficients for each species, one in the temperature range 0° to $1000^\circ K$ and the other from 1000° to $6000^\circ K$. 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:

$$Q_R = C_p T_{FP} \quad (10)$$

$$Q_R = C_v T_{FV} \quad (11)$$

$$T_{FV} = C_p / C_v T_{FP} = \gamma T_{FP} \quad (12)$$

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

$$F_p = \frac{R}{M} T_{FV} \quad (13)$$

where $R = 2780 \text{ ft-lbs/lb-mole-}^\circ K$

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 temperatures 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 ₂ H 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 ₈	+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 ₅ 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:

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

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

$$\mu_{MIX} = \sum_{i=1}^n \left(x_i \mu_i \right) \left(\sum_{j=1}^n x_j \phi_{ij} \right) \quad (15)$$

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

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

The thermal conductivity of a species is given as:

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

The mixture value is given as

$$K_{MIX} = \sum_{i=1}^n \left(x_i K_i \right) \left(\sum_{j=1}^n x_j \phi_{ij} \right) \quad (18)$$

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 constituents.

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 ₂ O	18.0	2.824	230.9

Table IV consists of the $\Omega - \frac{KT}{\epsilon}$ relations needed for the solution of Equations (14) and (17). The first column contains values for the relatively non-polar species such as H₂, N₂, CO, and CO₂, while the second column has a corrected value for the highly polar H₂O.

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 $C_4H_3O \cdot CH_2OH$ to represent its structure, must be treated as though it were $C_5H_6O_2$ or $O_2H_6C_5$, 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 79 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 OMIT and INSERT cards is completely optional; however when used, each card must contain either the code word OMIT 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 THERMO 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 FORTRAN 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 FORTRAN 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 $C_p = A_1 + A_2 T + A_3 T^2 + A_4 T^3 + A_5 T^4$. 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 indicator
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
IDDEBUG	Logical	False	Print intermediate output

TABLE VI. VARIABLES IN RKTNP NAMELIST			
Variable Name	Variable Type	Value Unless Set Differently	Definition
EQL	Logical	True	Gun propellant performance assuming equilibrium composition to be calculated
FRQZ	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.

Case 100				
	Tv	Fp	γ	Mw
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 OMIT or INSERT cards are used.

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		
T 11.0				.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		ENTHALPY		STATE		TEMP	
						(SEE NOTE)		CAL/MOL				DEG K	
FUEL C 24.00000 H 29.50000 O 41.30000 N 10.60000						1.00000		-643100.000				298.00	
OXIDANT C 12.00000 H 11.00000 N 1.00000						.33000		27600.000				298.00	
OXIDANT C 2.00000 H 14.00000 O 6.00000 N 4.00000						.67000		-66300.000				298.00	
O/F = .0204						PERCENT FUEL = 98.0000		EQUIVALENCE RATIO = 1.5547		DENSITY = 0.0000			
CHARGER													
CHAMBER	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
1.000	1.788	1.200	1.400	1.800	2.000	3.000	4.000	5.000	10.000	18.000	58.000	58.000	58.000
340.2	190.3	283.5	243.0	212.5	170.1	113.4	85.06	68.05	34.02	5.003			
2713	2443	2625	2553	2491	2391	2217	2101	2015	1766	1227			
-562.7	-681.0	-601.2	-632.7	-659.3	-702.4	-776.2	-825.3	-861.6	-965.0	-1189.2			
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													
(DLV/DLP)T	25.125	25.137	25.130	25.133	25.135	25.138	25.141	25.143	25.143	25.144	25.148		
(DLV/DLP)P	-1.00052	-1.00022	-1.00040	-1.00032	-1.00026	-1.00019	-1.00010	-1.00007	-1.00005	-1.00003	-1.00003		
CP, CAL/(G) (K)	1.0096	1.0040	1.0074	1.0058	1.0047	1.0033	1.0017	1.0010	1.0007	1.0003	1.0037		
GAMMA (ST)	.4447	.4313	.4398	.4362	.4334	.4294	.4239	.4209	.4191	.4152	.4239		
SON VEL./M/SEC	1.2206	1.2263	1.2226	1.2241	1.2253	1.2272	1.2300	1.2316	1.2320	1.2352	1.2307		
MACH NUMBER	1046.8	995.0	1030.5	1016.7	1004.8	985.1	949.7	925.1	906.2	849.4	786.6		
VEL. FT/SEC	0.00	1.000	.951	.753	.895	1.098	1.408	1.603	1.745	2.168	3.240		
VISC, G/CM-SEC	.000795	.000738	.000777	.000762	.000749	.000727	.000690	.000665	.000656	.000591	.000468		
C, CAL/G-SEC-K	.000300	.000281	.000294	.000289	.000285	.000278	.000266	.000256	.000251	.000234	.000201		
T, CV, DEG K	3312												
IMPETUS	36654.8.												
CSTAR, FT/SEC													
CF	4760	4760	4760	4760	4760	4760	4760	4760	4760	4760	4760	4760	4760
AE/AT	.686	.391	.528	.528	.820	.745	.921	.921	1.022	1.090	1.265	1.378	1.378
IVAG, LB-SEC/LB	1.000	1.266	1.065	1.065	1.011	1.008	1.134	1.134	1.292	1.452	2.194	8.385	8.385
I, LB-SEC/LB	184.2	213.9	190.5	185.1	185.1	184.8	192.3	199.0	204.2	219.2	219.2	251.5	251.5
	101.5	57.9	78.1	78.1	91.7	110.3	136.3	151.2	161.3	187.1	233.5	233.5	233.5

TABLE VIII. Concluded

MOLE FRACTIONS													
CH ₄	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000	.00000
CO	.40186	.39739	.40060	.39943	.39834	.39637	.39229	.38996	.38611	.37568	.33827	.00000	.00000
CO ₂	.13746	.14236	.13866	.14019	.14130	.14339	.14339	.13991	.13976	.16431	.26966	.00000	.00000
H	.00104	.00046	.00082	.00066	.00054	.00039	.00020	.00012	.00000	.00002	.00000	.00000	.00000
H ₂	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00000	.00000	.00000	.00000	.00000
H ₂ O	.00016	.00066	.00013	.00011	.00009	.00007	.00004	.00002	.00002	.00001	.00000	.00000	.00000
NH ₃	.10392	.10883	.10739	.10664	.10781	.10990	.11415	.11753	.12044	.13101	.17615	.00000	.00000
N ₂	.23507	.23088	.23392	.23283	.23180	.22989	.22585	.22253	.21968	.20916	.16394	.00000	.00000
NO	.00003	.00003	.00003	.00003	.00003	.00003	.00002	.00002	.00002	.00002	.00002	.00002	.00002
N ₂ O	.00005	.00001	.00004	.00002	.00002	.00001	.00000	.00000	.00000	.00000	.00000	.00000	.00000
OH	.11974	.11983	.11976	.11980	.11982	.11984	.11986	.11987	.11987	.11987	.11989	.00000	.00000
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .00005 FOR ALL ASSIGNED CONDITIONS	.00061	.00019	.00043	.00032	.00024	.00015	.00006	.00003	.00001	.00000	.00000	.00000	.00000
C													
C ₂ H ₄	C ₂ H ₆	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆	C ₂ H ₂	C ₂ H ₄	C ₂ H ₆
NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂	NH ₂
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													

THEORETICAL GUN PROPELLANT PERFORMANCE ASSUMING EQUILIBRIUM COMPOSITION DURING EXPANSION

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TABLE IX. Concluded

[illegible]

25	C	CH	CH ₂	CH ₃	CH ₄	CH ₅	CH ₆	CH ₇	CH ₈	CH ₉	CH ₁₀	CH ₁₁	CH ₁₂	CH ₁₃	CH ₁₄	CH ₁₅	CH ₁₆	CH ₁₇	CH ₁₈	CH ₁₉	CH ₂₀	CH ₂₁	CH ₂₂	CH ₂₃	CH ₂₄	CH ₂₅	CH ₂₆	CH ₂₇	CH ₂₈	CH ₂₉	CH ₃₀	CH ₃₁	CH ₃₂	CH ₃₃	CH ₃₄	CH ₃₅	CH ₃₆	CH ₃₇	CH ₃₈	CH ₃₉	CH ₄₀	CH ₄₁	CH ₄₂	CH ₄₃	CH ₄₄	CH ₄₅	CH ₄₆	CH ₄₇	CH ₄₈	CH ₄₉	CH ₅₀	CH ₅₁	CH ₅₂	CH ₅₃	CH ₅₄	CH ₅₅	CH ₅₆	CH ₅₇	CH ₅₈	CH ₅₉	CH ₆₀	CH ₆₁	CH ₆₂	CH ₆₃	CH ₆₄	CH ₆₅	CH ₆₆	CH ₆₇	CH ₆₈	CH ₆₉	CH ₇₀	CH ₇₁	CH ₇₂	CH ₇₃	CH ₇₄	CH ₇₅	CH ₇₆	CH ₇₇	CH ₇₈	CH ₇₉	CH ₈₀	CH ₈₁	CH ₈₂	CH ₈₃	CH ₈₄	CH ₈₅	CH ₈₆	CH ₈₇	CH ₈₈	CH ₈₉	CH ₉₀	CH ₉₁	CH ₉₂	CH ₉₃	CH ₉₄	CH ₉₅	CH ₉₆	CH ₉₇	CH ₉₈	CH ₉₉	CH ₁₀₀
	CH ₂	CH ₃	CH ₄	CH ₅	CH ₆	CH ₇	CH ₈	CH ₉	CH ₁₀	CH ₁₁	CH ₁₂	CH ₁₃	CH ₁₄	CH ₁₅	CH ₁₆	CH ₁₇	CH ₁₈	CH ₁₉	CH ₂₀	CH ₂₁	CH ₂₂	CH ₂₃	CH ₂₄	CH ₂₅	CH ₂₆	CH ₂₇	CH ₂₈	CH ₂₉	CH ₃₀	CH ₃₁	CH ₃₂	CH ₃₃	CH ₃₄	CH ₃₅	CH ₃₆	CH ₃₇	CH ₃₈	CH ₃₉	CH ₄₀	CH ₄₁	CH ₄₂	CH ₄₃	CH ₄₄	CH ₄₅	CH ₄₆	CH ₄₇	CH ₄₈	CH ₄₉	CH ₅₀	CH ₅₁	CH ₅₂	CH ₅₃	CH ₅₄	CH ₅₅	CH ₅₆	CH ₅₇	CH ₅₈	CH ₅₉	CH ₆₀	CH ₆₁	CH ₆₂	CH ₆₃	CH ₆₄	CH ₆₅	CH ₆₆	CH ₆₇	CH ₆₈	CH ₆₉	CH ₇₀	CH ₇₁	CH ₇₂	CH ₇₃	CH ₇₄	CH ₇₅	CH ₇₆	CH ₇₇	CH ₇₈	CH ₇₉	CH ₈₀	CH ₈₁	CH ₈₂	CH ₈₃	CH ₈₄	CH ₈₅	CH ₈₆	CH ₈₇	CH ₈₈	CH ₈₉	CH ₉₀	CH ₉₁	CH ₉₂	CH ₉₃	CH ₉₄	CH ₉₅	CH ₉₆	CH ₉₇	CH ₉₈	CH ₉₉	CH ₁₀₀		

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												
OXIDANT C	4.00000	H	8.00000	O	8.00000	N	8.00000					
FUEL C	7.00000	H	11.00000	O	.20000	N	.02000					
O/F= 5.5667 PERCENT FUEL= 15.0000 EQUIVALENCE RATIO= 2.7550 DENSITY= 0.0000												
								WT FRACTION	ENTHALPY	STATE	TEMP	DENSITY
								(SEE NOTE)	CAL/MOL		DEG K	G/CC
								1.00000	17900.000		298.00	-0.0000
								1.00000	-5000.000		298.00	-0.0000
CHAMBER												
PC/P	1.000	THROAT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT	EXIT
P, ATM	340.2	187.0	1.019	1.200	1.400	2.000	3.000	4.000	5.000	10.000	60.000	
T, CP, DEG K	1995	1758	1918	263.5	243.0	212.6	170.1	113.4	68.05	34.02	5.003	
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, VOL WT												
(OLV/DLP) T	18.902	19.006	18.925	18.950	18.976	19.030	19.163	19.284	19.392	19.796	21.091	
(OLV/DLP) P	-1.01474	-1.02159	-1.01644	-1.01815	-1.01982	-1.02299	-1.02975	-1.03507	-1.03932	-1.05817	-1.07938	
CP, CAL/(G)(K)	1.0946	1.1603	1.1127	1.1309	1.1409	1.1639	1.2631	1.3303	1.3876	1.7060	2.2655	
GAMMA (S)	.5308	.5951	.5452	.5607	.5769	.6103	.6929	.7693	.8383	1.3712	2.3570	
SON VEL, M/SEC	1.2863	1.2791	.2854	1.2837	1.2817	1.2769	1.2642	1.2531	1.2438	1.1703	1.1394	
MACH NUMBER	1062.5	991.7	1040.8	1022.5	1006.7	980.7	934.5	903.3	880.2	809.4	693.4	
VEL, FT/SEC	0.0	3253.6	1837.3	2474.8	2903.8	3584.2	4293.7	4752.8	5084.5	5862.9	7351.1	
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.												
CSLAR, FT/SEC												
CF	.703	.397	.535	.535	.628	.753	.928	1.027	1.095	1.267	1.591	
AT/AT	1.000	1.290	1.072	1.014	1.014	1.006	1.123	1.279	1.431	1.704	2.087	
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	97.1	76.9	90.3	108.3	138.5	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	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
CH3	.00003	.00001	.00002	.00002	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001
CH4	.00418	.00735	.00494	.00571	.00649	.00605	.00617	.00610	.00603	.00603	.00603	.00603	.00603	.00603	.00603
CO	.00002	.00490	.00408	.00393	.00348	.00443	.00471	.00471	.00471	.00471	.00471	.00471	.00471	.00471	.00471
CO2	.00566	.00741	.00608	.00650	.00693	.00780	.00892	.00992	.01194	.01263	.01301	.01301	.01301	.01301	.01301
C2H2	.00002	.00001	.00002	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001
C2H4	.00002	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001
H	.00005	.00001	.00003	.00002	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001	.00001
HCN	.00136	.00074	.00114	.00098	.00084	.00067	.00067	.00067	.00067	.00067	.00067	.00067	.00067	.00067	.00067
HCO	.00007	.00002	.00005	.00004	.00003	.00003	.00002	.00002	.00002	.00002	.00002	.00002	.00002	.00002	.00002
H2	.34336	.33076	.34237	.34127	.34009	.33764	.33162	.32616	.32141	.31656	.31141	.30656	.30171	.29686	.29201
H2O	.02193	.02248	.02165	.02105	.02210	.02266	.02413	.02545	.02656	.02743	.02829	.02915	.03001	.03087	.03173
NH3	.00065	.00056	.00062	.00060	.00057	.00054	.00049	.00045	.00042	.00039	.00036	.00033	.00030	.00027	.00024
N2	.21627	.21782	.21806	.21704	.21742	.21814	.21982	.22129	.22259	.22318	.22359	.22398	.22437	.22476	.22515
ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .00005 FOR ALL ASSIGNED CONDITIONS															
C	CH	CH2	CN	CN2	C2	C2H	C2H2	C2H4	C2H6	C2N2	C2O	C2O2	C2O4	C2O6	C2O8
C3	H2O2	H2O2(l)	H2O2(s)	N	NH	NH2	NH3	NH4	NH5	NH6	NH7	NH8	NH9	NH10	NH11
N2H4	N2O	N2O2	O	OH	O2	O3	O4	O5	O6	O7	O8	O9	O10	O11	O12
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 = 500.0 PSIA

CASE 136 PROPELLANT IS ROX-TAG NITRATE

[illegible]

0/F=	2.3333	PERCENT FUEL=	30.0000	EQUIVALENCE RATIO=	2.6026	DENSITY=	0.0000
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[illegible][illegible]

HOLE FRACTIONS

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

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

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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	900	1000				
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				
1000	1100	1200	1300	1400	1500	1600	1700	1800	1900	2000	2100	2200
3000	3100	3200	3300	3400	3500	3600	3700	3800	3900	4000	4100	4200
5000	5100	5200	5300	5400	5500	5600	5700	5800	5900	6000		
14.117	14.211	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	19.234	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	95.383	95.677	95.960	96.238	96.511	96.779	97.043	97.301	97.556			
97.806												

TABLE XIII. THERMO DATA OUTPUT FORMAT FOR TITANIUM DIOXIDE

TITANIUM DIOXIDE (TiO2) IDEAL GAS

HO = -62000.0

VALUES OF G
COEFFICIENTS ARE

36725340E+01	10003020E-01	11120307E-04	49403359E-08	67934354E-12	32588921E+05	79567663E+01
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-33589155E-02	-54917462E-02	-15152376E-01				
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T	CP	CCP	HT	CHT	ST	GST	DCP	DHT	DST
---	----	-----	----	-----	----	-----	-----	-----	-----

298.	10.838	10.838	0.000	0.100	56.146	56.146	.000	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.	12.540	12.540	2.376	2.377	62.194	62.194	.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	13.958	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	-50104624E-06	.85525393E-10	-.53125222E-14	-.32336518E+05	-.81070897E+01
--------------	--------------	---------------	---------------	----------------	----------------	----------------

95760211E-01	22837632E-01	10773479E+00				
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T	CP	CCP	HT	CHT	ST	GST	DCP	DHT	DST
---	----	-----	----	-----	----	-----	-----	-----	-----

1000.	14.117	14.117	9.138	9.138	71.506	71.506	.000	.000	.000
1100.	14.241	14.214	18.556	18.555	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	17.423	17.415	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	28.046	28.037	83.586	83.577	.030	.008	.009
2400.	14.754	14.784	29.515	29.515	84.213	84.206	.030	.004	.007
2500.	14.765	14.795	30.985	30.984	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	14.808	33.968	33.964	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	50.257	91.017	91.013	.016	.006	.004
3900.	14.846	14.829	51.736	51.740	91.402	91.399	.017	.004	.003
4000.	14.849	14.832	53.220	53.220	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	56.198	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	60.644	60.644	93.528	93.522	.006	.001	.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	.002	.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.	14.875	14.847	82.955	82.960	97.806	97.802	.032	.005	.004

TABLE XIV. DATA TAPE FORM FOR THERMØ DATA OUTPUT

T102	J 6/70T1	10	200	000	06	299.000	6000.000	1
C.62406876E+01	0.12846967E-02	-0.50184624E-06	0.85525393E-10	-0.53125222E-14				2
-0.3336518E+05	0.81878897E+01	0.30725348E+01	0.10883020E-01	-0.11120307E-04				3
0.49483359F-08	-0.67934354F-12	-0.32508921E+05	0.79567663F+01					4

SECTION V

THERMO DATA PROGRAM

The program (Appendix II) to fit the tabular JANAF thermochemical data to the Lewis polynomial is relatively simple and straightforward. 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 TiO_2 . 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 TiO_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.

APPENDIX I
LEWIS PROGRAM LISTING

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		PROGRAM P1712	INPUT, OUTPUT, TAPES=INPUT, TAPES=OUTPUT, TAPES=4, TAPES=9	P1712	00002
		I E R P G	REFERENCE PROGRAM ODE	P1712	00003
		C	DECK SEQUENCED BY SUBROUTINE	P1712	00004
		C	THERMODYNAMIC DATA FOLLOWS SOURCE DECK	P1712	00005
05		C	DATA FOR TEST CASES FOLLOWS THERMODYNAMIC DATA	P1712	00006
		C	PROGRAM USES TAPE UNIT 4 FOR THERMO DATA	P1712	00007
		C		P1712	00008
		C	ODE ICRPG REFERENCE PROGRAM	P1712	00009
		C		P1712	00010
10		C	MAIN PROGRAM	P1712	00011
		C		P1712	00012
		C		P1712	00013
		C	DOUBLE PRECISION G,X	P1712	00014
		C	INTEGER DATA, ORIT, ENSERT, REAC, BLANK, THRM, END, SUB	P1712	00015
15		C	LOGICAL HP, SP, TP, IDEBUG, NEMR, IONS, MOLES, FROZ, EQL, PSIA, RKT	P1712	00016
		C	LOGICAL SHOCK, MPMG, PASCAL, EV, IC, DETN, CPCVFR, CPCVEG, SIUNIT, EUNITS	P1712	00017
		C		P1712	00018
		C	DIMENSION OMIT(2,3), NCD(4), ENSERT(13,3), LH(2), LVP(2), LVM(2)	P1712	00019
		C	COMMON/POINTS/HSUT(13), SSUM(13), CPR(13), DUTP(13), DULVPT(13)	P1712	00020
20		1	GAMMAS(13), P(26), T(26), V(13), PPP(13), MM(13), SONVEL(13), TIT(13)	P1712	00021
		2	TOTN(13)	P1712	00022
		C	COMMON/SPECES/CDEF(2,7,150), S(150), EN(150,13), ENLN(150), H3(150)	P1712	00023
		1	CELN(150), A(15,150), SUB(150,3), IUSE(150), TEMP(50,2)	P1712	00024
		C	COMMON/MISC/ENNSUMN, IT, SO, ATOM(3,101), LLMT(15), BU(15), BOP(15,2)	P1712	00025
25		1	TH, TLOW, THIU, THIS, PP, CPSUM, OF, EQRT, FPCT, R, R, RSUBU, AG(2), AM(2)	P1712	00026
		2	HPP(2), RHU(2), VMIN(2), VPLS(2), MP(2), DATA(22), NAME(15,5)	P1712	00027
		3	ANUM(15,5), PECHT(15), ENTH(15), FAZ(15), RTEHP(15), FOX(15), DENS(15)	P1712	00028
		4	RHOP, KYM(15), LCN, JANF	P1712	00029
		C	COMMON/DOUBLE/ G(20,21), X(20)	P1712	00030
30		C	COMMON/INDEX/ IDEBUG, CONVG, TP, HP, SP, HPSP, TPSP, MOLES, NP, NT, NPI, L, NS,	P1712	00031
		1	XMAT, INAT, IGIN, J, NMOT, IP, NEMR, NSUB, NSUP, ITN, CPCVFR, CPCVEU	P1712	00032
		2	IONS, NC, NSERT, JSOL, JULIQ, KASE(14), NREAC, IC, IO2	P1712	00033
		C	COMMON/PERF/PCP(26), VRQC(13), SPIH(13), VAGI(13), SUBAR(13), SUPAR(13)	P1712	00034
35		1	CPRF(13), AEAT(13), CSTR, EQL, FROZ, SSO	P1712	00035
		C		P1712	00036
		C	EQUIVALENCE (OMIT, ENLN), (ENSERT, EN(1,3))	P1712	00037
		C		P1712	00038
		C	DATA MIT/4HOMIT/, BLANK/1H /, PSIA/4HPSIA/, REAC/4HREAC/.	P1712	00039
40		1	INPUT/4HINPUT/, IE/1HE/, INSERT/4HINSE/, THRM/4HTHER/, END/3HEND/	P1712	00040
		C	DATA LH/4HL/, CA, 4HL/G /, LVP/2HJV/, LH /, LVM/2HVM/, LH /, NMLT/4HNMLT/	P1712	00041
		C	NAMELIST/INPT2/JANF, P, T, EQRT, OF, FPGI, FA, TP, HP, SP, RKT	P1712	00042
		1	PSIA, MPMG, SHOCK, IONS, EV, V, DETN, CPCVFR, CPCVEG, IDEBUG	P1712	00043
		2	SIUNIT, EUNITS	P1712	00044
45		C	TLOW = 0.	P1712	00045
		C	NEMR = .FALSE.	P1712	00046
		C	DO 399 I=1,15	P1712	00047
		C	DO 398 J=1,150	P1712	00048
50		C	A(I,J) = 0.0	P1712	00049
		C	398 CONTINUE	P1712	00050
		C	399 CONTINUE	P1712	00051
		C		P1712	00052
		C		P1712	00053
		C		P1712	00054


```

300 CONTINUE
    V1 = 0.
    V2 = 0.
    RHOP = 0.
    KASE = 0
    IP = .FALSE.
    HP = .FALSE.
    SP = .FALSE.
    RKT = .FALSE.
    CPCVR = .FALSE.
    CPCVEJ = .FALSE.
    SHOCK = .FALSE.
    DETN = .FALSE.
    EV = .FALSE.
    PASCAL = .FALSE.
    MMHG = .FALSE.
    PSIA = .FALSE.
    R = 1.987165
    TR = 418.7
    SIUNIT = .FALSE.
    EUNITS = .FALSE.
    IONS = .FALSE.
    IDEBUG = .FALSE.
    FA = 0.
    UF = 0.
    EGRAT = 0.
    FPCT = 0.
    EGL = .TRUE.
    READ(5,303)KASE
303 FORMAT(13A5,A2)
    K2U(5,INPT2)
    DO 305 I=1,26
    IF(P(I).EQ.0.) GO TO 322
    NP = I
    IF (MMHG) P(NP) = P(NP)/760.
    IF (PASCAL) P(NP) = P(NP)/101325.
    IF P(SIA)
    P(NP) = P(NP)/14.696056
305 CONTINUE
322 IF (FA.NE.0.) OF = 1./FA
    IF (EORAT.EQ.0.) GO TO 725
    OF = (-EORAT*VMIN(2)-VPLS(2))/(VPLS(1)+EGRAT*VHIN(1))
    GO TO 727
725 IF (OF.NE.0.) GO TO 727
    IF (FPCT.EQ.0.) GO TO 9051
    OF = (1.-FPCT)/FPCT
    GO TO 727
9051 WRITE(6,724)
724 FORMAT(48HNO INPT2 VALUE GIVEN FOR OF, EGRAT, FA, OR FPCT )
727 WP(1) = OF
    WP(2) = 1.
    SUM = WP(1)+WP(2)
    FPCT = 100.*WP(2)/SUM

```

```
160 IF (EORAT.NE.0.) GO TO 745
    V2 = (WP(1)*VMIN(1)+WP(2)*VMIN(2))/SUM
    V1 = (WP(1)*VPLS(1)+WP(2)*VPLS(2))/SUM
    IF (V2.NE.0.) EORAT=ABS(V1/V2)
    745 DO 747 I=1,L
        80(I) = (WP(1)*BOP(I,1)+WP(2)*BOP(I,2))/SUM
    747 CONTINUE
    IF (EORAT.EQ.1.) EORAT= 1.000005
    IF (.NOT.(IONS.OR.L.NI(L).EQ.1E) ) GO TO 748
    L = L+1
    LL*1(L) = IE
    80(L) = 0.
    748 HSUB0 = (WP(1)*HPP(1)+WP(2)*HPP(2))/SUM
    WRITE (6,10PT2)
    WRITE (6,752)KASE
    752 FORMAT(1H0,13A6,A2/)
    WRITE (6,770)
    770 FORMAT(1H0,17X,4HFUEL,13X,7HOXIDANT,12X,7HMIXTURE //)
    780 FORMAT(1H0,24X,5E15,87)
    WRITE (6,730) LH,HPP(2),HPP(1),HSUB0,LVP,VPLS(2),VPLS(1),V1,
    1LVM,VMIN(2),VMIN(1),V2
    HSUB0 = HSUB0/R
    WRITE (6,785)
    785 FORMAT(8H ATOMS/G )
    RHOP = WP(2)*RH0(1)+WP(1)*RH0(2)
    IF (RHOP.NE.0.) RHOP = (WP(1)+WP(2))*RH0(1)*RH0(2)/RHOP
    795 IF (NEWR) CALL SEARCH
    701 = L+1
    IF (NC.EQ.0) GO TO 790
    80 302 J=1,NS
    IF (IUSE(J).EQ.0) GO TO 302
    IF (IUSE(J).GT.0) IUSE(J) = -IUSE(J)
    IF (INSERT.EQ.0) GO TO 302
    00 301 I=1,MSERT
    IF (SUB(J,1).NE.INSERT(1,I)) GO TO 301
    IF (SUB(J,2).NE.INSERT(2,I)) GO TO 301
    IF (SUB(J,3).NE.INSERT(3,I)) GO TO 301
    INSERT(1,I) = 0.
    IQ1= I01+1
    IUSE(J) = -IUSE(J)
    301 CONTINUE
    302 CONTINUE
    NSERT = 1
    790 IIN= 35
    IC = .FALSE.
    PP = NS
    NPT = 1
    ENN = 1
    SUPN = ENN
    XI = NS - NC
    XI = ENN/XI
    XLN = AL9G(XI)
```

```

215      UU 432 J=I,NS
          IF(IUSE(J),50,-10000) IUSE(J)=0
          EN(J,1) = 0,
          ENLN(J)=0,
          IF (IUSE(J),NE,0) GO TO 432
          EN(J,1) = XI
          ENLN(J) = XLN
220      432 CONTINUE
          JSCL = 0
          JLIQ = 0
          IF(OETN) CALL DETON
          IF(RKT) CALL ROCKET
          IF (TP) CALL HOLIER
          IF (WP) CALL CMBSYN
          500 CONTINUE
          GC TO 1
          END
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```

P1712 00214
P1712 00215
P1712 00216
P1712 00217
P1712 00218
P1712 00219
P1712 00220
P1712 00221
P1712 00222
P1712 00223
P1712 00224
P1712 00225
P1712 00226
P1712 00227
P1712 00228
P1712 00229
P1712 00230

[illegible]

SUBROUTINE CMO3YN

C

COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),OLVTP(13),OLVPI(13)

1,CAM4AS(13),P(26),T(26),V(13),PPP(13),N(13),SONVEL(13),ITT(13)

2,TTN(13)

COMMON/SPFGES/CGEF(2,7,150),S(150),EV(150,13),ENLN(150),P(150)

1,TELT(150),TA(15,150),SUB(150,3),IUSE(150),TEPR(50,2)

COMMON/MISC/ENN,SUIN,TT,S0,ATOM(3,101),LLMT(15),BU(15),BOP(15,2)

1,TH,TLOW,THIO,THIEM,PP,CPSUM,OF,EORAT,EPT,R,RR,HSUB0,AC(2),AM(2)

2,PPP(2),R4U(2),VMIN(2),VPLS(2),NP(2),DATA(22),NAME(15,5)

3,ANUM(15,5),PECT(15),CNTH(15),FAZ(15),ATENP(15),FOX(15),DEMS(15)

4,RHOP,R4W(15),TLN,JANF

COMMON/INDX/IDEBUG,CONVG,IP,WP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,

1,KMAT,IMAT,ICI,N,J,NOMIT,IP,NEMR,NSUB,NSUP,IFA,CPCVFR,CPCVEG

2,IONS,NG,NSERT,JSOL,JLIG,KASE(14),NREAC,IC,I02

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P1712 00313

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P1712 00315

P1712 00316

P1712 00317

P1712 00318

P1712 00319

P1712 00320

P1712 00321

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SUBROUTINE CPHS

COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),HQ(150)

1 .GELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)

COMMON/ SC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),80(15),80P(15,2)

1 .TM, .OK,THID,THIGH,PP,CPSUM,OF,FOUR,FPCIR,R,R,HSUB0,AC(2),AM(2)

2 .FPP(27),RHOT(27),VPLST(27),VPLST(2),DATA(27),NAME(15,5)

3 .ANUM(15,5),PECTH(15),FZ(15),RTEMP(15),FOX(15),DENS(15)

4 .RHOP,RMH(15),TLN,JANF

COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,

1 .KMAT,THAT,IQI,N,J,NOHIT,IP,NEHR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ

2 .IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAG,IC,IQ2

K = 1

IF (TT,LF,THID) K = 2

KK = 0

CPSUM=0.

90 IF (COEF(K,1,J),NE,0.) GO TO 97

IF (IUSE(J),LT,0) GO TO 100

KK = K

K = 1

IF (KK,EQ,1) K = 2

97 CONTINUE

IF (JANF,EQ, 0) GO TO 98

S(J)=COEF(K,1,J) - TLN*COEF(K,7,J) - TLN*COEF(K,5,J)/2 - TT/TT

1 + ((COEF(K,4,J)/3.0 - TT*COEF(K,3,J)/2.0) * TT + COEF(K,2,J)) * TT

HQ(J) = (((COEF(K,4,J)/4.0) * TT + COEF(K,3,J)/3.0) * TT + COEF(K,2,J) / 2.0) *

1 TT + COEF(K,1,J) - (COEF(K,5,J)/TT - COEF(K,6,J))/TT

CPSUM=CPSUM + ((COEF(K,4,J) * TT + COEF(K,3,J)) * TT + COEF(K,2,J)) * TT

1 + COEF(K,1,J) - COEF(K,5,J)/TT + COEF(K,6,J) * EN(J,NPT)

GO TO 99

98 S(J) = (((COEF(K,5,J)/4.0) * TT + COEF(K,4,J)/3.0) * TT + COEF(K,3,J)/2.0

1) * TT + COEF(K,2,J)) * TT + COEF(K,1,J) - TLN + COEF(K,7,J)

HQ(J) = (((COEF(K,5,J)/5.0) * TT + COEF(K,4,J)/4.0) * TT + COEF(K,3,J)/3.0

1) * TT + COEF(K,2,J)/2.0) * TT + COEF(K,1,J) + COEF(K,6,J) / TT

CPSUM= CPSUM + (((COEF(K,5,J) * TT + COEF(K,4,J)) * TT + COEF(K,3,J)) * TT

1 + COEF(K,2,J) * TT + COEF(K,1,J)) * EN(J,NPT)

99 CONTINUE

IF (KK,EQ,0) C. TO 100

K = KK

KK = 0

100 IF (J,EQ,NS) GO TO 200

J=J+1

GO TO 90

200 RETURN

ENC

SUBROUTINE DETON									
C						P1712	00401		
C						P1712	00402		
C						P1712	00403		
C						P1712	00404		
05						P1712	00405		
						P1712	00406		
C						P1712	00407		
						P1712	00408		
C						P1712	00409		
						P1712	00410		
10						P1712	00411		
						P1712	00412		
						P1712	00413		
						P1712	00414		
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50						P1712	00450		
						P1712	00451		
						P1712	00452		
						P1712	00453		

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55      7 IF (AM(1).NE.0.0) AND. AM(2).NE.0.0) GO TO 4
      AM1 = AM(2)
      IF (AM(2).EQ.0.0) AM1 = AM(1)
      GO TO 9
      4 AM1 = (MP(1)+MP(2))*AM(1)*AM(2)/(MP(2)*AM(1)+MP(1)*AM(2))
      3 CONTINUE
      60 DO 902 IT=1,N1
      T1 = T/IT
      IF (T1)
      IF (CALCH) CALL HCALC
      CP1 = (MP(1)*AC(1)+MP(2)*AC(2))/(MP(1)+MP(2))
      65 DO 902 IP=1,NP
      P1 = P(TP)
      H1(NP1) = HSUB0
      TUB(NP1)=T1
      PUR(NP1)=P1
      CP(NP1) = CP1*Q
      70 ITR= 0
      TT= 3600.
      PP1= 15.
      PP= PP1*P1
      HSUB0 = H1(NP1)/R + .75*TT*PP1/AM1
      TP = .FALSE.
      HP = .TRUE.
      CALL EOLDRM
      75 HSUB0 = H1(NPT)
      HP= .FALSE.
      IF (TT.EQ.0.) GO TO 1000
      GAP= GAMMAS(NPT)
      TT1= TT/TT1
      II= 0
      85 TEM=TT1-.75*PP1/(CPR(NPT)*AM1)
      AMH=MH(NPT)/AM1
      IF (IDEBUG) WRITE(6,190)
      190 FORMAT(33HDETONATION VELOCITY CALCULATIONS /11X,4HP/P1,17X,4HT/11
      1)
      IF (IDEBUG) WRITE(6,203) II,PP1,TT1
      C
      200 DO 202 II=1,4
      ALFA=AMH/TT1
      PP1= (1.+GAM)* (1.+(1.-G.*GAM*ALFA/(1.+GAM))*2)**.5)/(2.*GAM*.LFA)
      RK=PP1*ALFA
      TT1= TEM+.5*PP1*GAM*(RK*RK-1.)/(AM1*CPR(NPT)*RK)
      95 IF (IDEBUG) WRITE(6,203) II,PP1,TT1
      203 FORMAT (15,2E20.8)
      202 CONTINUE
      TP= .TRUE.
      100 TT= T1*TT1
      AM1 = PP1*AMH/TT1
      C
      205 ITR= ITR+1
      PP= PP1*PP1
      CALL EOLDRM

```

```
IF (NPT.EQ.0) GO TO 1000
*F (TT.EQ.0) GO TO 860
GAM= GAMAS(NPT)
IF (CPCVFR) GAM= CPRF(NPT) / (CPRF(NPT)-1./WM(NPT))
IF (CPCVEU) GAM= -GAMAS(NPT)*DLVPT(NPT)
AMP= AM(NPT)/AM1
KRI= PP1*AM/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)*(RSUM(NPT)-HI(NPT)/R)/TT-.5*GAM*(RR1*RR1-1.)
X1= XX(Y)
X2= YY(Z)
ALAM= 1.
TE4= X1
IF (TEM.LI.0.) TEM= -TEM
IF (X2.GT.TEN) TEN=X2
IF (-X2.GT.TEN) TE4= -X2
IF (TEM.GT.0.4) ALAM=.4/TEM
PP1= PP1*EXP(X1*ALAM)
TT1= TT1*EXP(X2*ALAM)
TT= TT1
US= (RR*GAM*TT/WM(NPT))**.5
UD= RR1*UG
IF (IDERUG) WRITE(6,10) ITR
10 FORMAT (21H0 ITERATION NUMBER=12 )
IF (ICEBUG) WRITE(6,30) PP1,TT1,RR1,X1,X2,US
30 FORMAT (6X,4HP/PP1,10X,1H= E20.8/6X,4HT/TT1, 10X,1H= E20.8/6X,8HRH0/RM
101,6X,1H= E20.8/6X,11HDEL IN P/PP1,3X,1H=E20.8/6X,11HDEL IN T/TT1,3X
2,1H=E20.8/6X,2HUS,12X,1H=E20.8)
CONVERGENCE TEST
IF (ITR.LE.10 .AND. TEM.GT.0.5E-04) GO TO 205
KRM(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
150
C
C DERIVATIVES
41 IF (ICEBUG) WRITE(5,55)
55 FORMAT (17H0 DERIVATIVE OF:13X,AMEN P,10X,AMEN T,10X,2HUD,
1
/3X,2HBY )
B1= 1./PP1-GAM*RR1
B2= GAM*RR1**2
X1= XX(Y)
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160 X2 = YY(2)
    AA = .5*(1.-OLVPT(NPT))
    88 = .5*OLVPT(NPT)
    OUC = UD*(AA*X1+BB*X2-1.)
    X1 = X1-1.0
    165 IF(IDERUG) WRITE(6,81) X1,X2,DUD
    81 FORMAT(6X,13HCP(NPT) AT T1,M1,3X,1H=,3E17.8)
    B1 = GAM*RR1
    82 = -B1*RR1-MM(NPT)*CP(NPT)/(R*TT1)
    X1 = XX(Y)
    X2 = YY(Z)
    DUD = UD*(AA*X1+BB*X2+1.)
    X2 = X2-1.0
    175 IF(IDERUG) WRITE(6,84) X1,X2,DUD
    84 FORMAT(6X,16HINT1 AT P1,M1,3X,1H=3E17.8)
    B1 = 0.
    87 = -MM(NPT)/(R*TT1)
    X1 = XX(Y)+1000.
    X2 = YY(Z)+1000.
    DUD = UD*(AA*X1+BB*X2)
    180 IF(IDERUG) WRITE(6,85) X1,X2,DUD
    85 FORMAT(6X,20HH1 AT T1,P1,M1 =3E17.8)
    C
    150 K = 0
    185 IF(17P.EQ.NPT.ND.IF-K-2.NF-OR.TT.EQ.0.) GO TO 830
    K = NPT
    IF(NPT.NE.13) GO TO 870
    C
    C OUTPUT
    C
    190 5 WRITE(6,5)
    5 FORMAT(1H1,42X,46HDETONTATION PROPERTIES OF AN IDEAL REACTING GAS )
    CALL OUT1
    WRITE(6,46)
    195 46 FORMAT(13H UNBURNED GAS//)
    FMT(4)=FMT13
    FMT(5)=F8
    FMT(7)=F4
    WRITE(6,FMT)FP1,FP(2),FB,FB,(PUB(J),J=1,NPT)
    FMT(7)=F2
    WRITE(6,FMT)FT1,FT(2),FB,FB,(TUB(J),J=1,NPT)
    WRITE(6,FMT)FM1,FM(2),FB,FB,(H1(J),J=1,NPT)
    80-56 I=.NPT
    V(I)=AM1
    SONVEL(I) = (RR*GM1(I)*TUB(I)/AM1)**.5
    205 56 CONTINUE
    FMT(7)=F3
    WRITE(6,FMT)FN1,F1(2),FM(3),FB,(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,FB,FB,(GM1(J),J=1,NPT)
    FMT(7)=F1
    WRITE(6,FMT){FL(I),I=1,4},{SONVEL(J),J=1,NPT}
```

```

215      WRITE(6,55)
55      FORMAT(11HBOURNED GAS//)
      FMT(4)=FMT(6)
      CALL OUT2
      WRITE(6,56)
68      FORMAT(22HDETENTIONATION PARAMETERS //)
      FMT(7)=F4
220      DO 70 I=1,NPT
          V(I)=PPF(I)/PUB(I)
          PCP(I)=IT(I)/TUB(I)
          SONVEL(I)=SONVEL(I)*RRHO(I)
70      CONTINUE
225      WRITE(6,FMT)FPP,FB,FB,FB,IV(I),J=1,NPT)
      WRITE(6,FMT)FIT,FB,FB,FB,PCP(J),J=1,NPT)
      DO 73 I=1,NPT
          V(I)=MM(I)/AM1
73      CONTINUE
      FMT(7)=F4
230      WRITE(6,FMT)FPM,FB,FB,FB,IV(I),J=1,NPT)
      WRITE(6,FMT)FRA,FR3,FB,FB,RRHO(J),J=1,NPT)
      WRITE(6,FMT)FMA,FMB,FB,FB,VMOC(J),J=1,NPT)
      FMT(7)=F1
235      WRITE(6,FMT) FUD,FL(2),FL(3),FL(4),(SONVEL(J),J=1,NPT)
          EQL=.TRUE.
      CALL OUT3
240      865 IF(K.EQ.0) GO TO 1000
          WRITE(6,865)
          868 FORMAT(1M1)
          NPT = 0
          870 NPT = NPT + 1
          C
          C      SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT
          C
245      DO 880 I = 1,NS
          EN(I,NPT) = EN(I,K)
          880 CONTINUE
          902 CONTINUE
250      1000 TP = .FALSE.
          RETURN
          ENC

```

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SUBROUTINE EQL82M FORTRAN EXTENDED VERSION 2.0

```

55      IF(IQ1) GO TO 171
      IF (.NOT. CONVG. OR .JSOL.EQ.0) GO TO 62
      ENSOL = EN(JSOL,NPT)
      EN(JSOL,NPT) = EN(JSOL,NPT) + EN(JLQ,NPT)
      IUSE(JLQ) = -IUSE(JLQ)
      IQ1 = IQ1 - 1
      DLVTP(NPT) = 0.
      CP3(NPT) = 0.
      GAPRAS(NPT) = 0.
      LOGV = .TRUE.
      62 CALL MATRIX
      NUMB = IYN - IYNB + 1
      IF(.NOT. CONVG) GO TO 67
      IF (LOGV.AND. JSOL.EQ.0) GO TO 63
      DO 182 I=1,L
      PRCH(I) = G(IQ1,I)
      70      182 CONTINUE
      IF (.NOT. LOGV) GO TO 67
      C
      C      LCGV = .TRUE. -- SET UP MATRIX TO SOLVE FOR DLVPT
      C
      75      63 G(IQ1,IQ2) = ENN
      IG = IQ1 - 1
      DO 777 I = 1,IQ
      G(I,IQ2) = G(I,IQ1)
      777 CONTINUE
      80      67 IF (.NOT. IOEBUG) GO TO 72
      WRITE(6,772) NUMB
      772 FORMAT (11H0 ITERATION ,I3.6X,7HMATRIX //)
      DO 911 I=1,IMAT
      911 WRITE (6,737) (G(I,K)*K=1,KMAT)
      72 IF (CONVG) IMAT=IMAT-1
      ITST = IMAT
      CALL MGAUSD
      IF (ITST.NE.IMAT) GO TO 774
      IF (.NOT. IOEBUG. OR. CONVG) GO TO 773
      90      WRITE (6,3737) (I=1,I1)
      3737 FORMAT (7H0PI ,9(A4.10X))
      WRITE (6,73) (X(I),I=1,IMAT)
      73 FORMAT (9E14.0)
      773- IF (.NOT. CONVG) GO TO 85
      IF (LOGV) GO TO 171
      95      174 SUP = 0.
      DO 175 J=1,L
      SUM = SUM + PRCH(J)*X(J)
      175 CONTINUE
      DLVTP(NPT) = 1. + G(IQ2,IQ1)/ENN - SUM/ENN - X(IQ1)
      CP3(NPT) = G(IQ2,IQ2)
      DO 176 J=1,IQ1
      CP3(NPT) = CP3(NPT) - G(IQ2,J)*X(J)
      176 CONTINUE
      LOGV = .TRUE.
      105      GO TO 62

```

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```

C
C SINGULAR MATRIX
C
110      774 IF(.NOT.CONVG) GO TO 775
        WRITE(6,172)
172      FORMAT(23HDERIVATIVE MATRIX SINGULAR )
        IC = .TRUE.
        GO TO 171
115      775 IF (.NOT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.IT.GT.100.) GO TO 371
        WRITE(6,874)
174      FORMAT(96HLOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
        196EN INCLUDED ON AN INSERT CARD, RESTART )
        GO TO 873
120      971 WRITE (6,74)
        74      FORMAT(16HOSINGULAR MATRIX)
        IF (IC) GO TO 973
        IF (ISING) GO TO 937
        NTZERO = 0
125      965 DO 970 JJ = 1, NS
        IF (IUSE(JJ)) 97C,968,967
        967 IF (EN(JJ,NPT).EQ.0.) GO TO 873
        GO TO 969
        969 IF (EN(JJ,NPT).NE.0.) GO TO 969
        EN(JJ,NPT) = SMALNC
        EN(JJ) = SMALC
        GO TO 970
        969 NTZERO = NTZERO+1
        970 CONTINUE
        IF (.NOT.IC) GO TO 971
        IC = .FALSE.
        GO TO 43
130      971 ISING = .TRUE.
        WRITE (6,776)
        776      FORMAT (9HRESTART)
        GO TO 43
        997 IF (NTZERO.NE.(L-1)) GO TO 873
        IF (FORMAT,GT.1.00001.0K) EORAT,LT,0.99999) GO TO 873
        EARN=0.
        NEN = 0
        DO 83 I=1,L
        JEN=0
        DO 80 J=1,NS
        IF (EN(J,NPT).EQ.0.) GO TO 88
        IF (A(I,J).EQ.0.) GO TO 83
        IF (JEN.NE.0) GO TO 83
        JEN = J
        80      CONTINUE
        NEN = NEN+1
        EN(JEN,NPT) = 0.06447413JEN)
135      83      CONTINUE
        IF (NEN.LT.NTZERO) GO TO 373
        CONVG = .TRUE.
        IC = .TRUE.

```

```
167 HSUM(NPT) = J.  
    DO 84 J=1,NS  
      IF (CN(J,NPT).EQ.0.) GO TO 84  
      ENN = EN(J,NPT)+ENH  
      TEP = EN(J,NPT)  
      ENLN(J) = ALOG(TEP)  
165 HSUM(NPT) = HSUM(NPT) + EN(J,NPT)*HU(J)  
    84 CONTINUE  
      TM = ALOG(PP/ENN)  
      GO TO 43  
170 85 ITNUM8= ITNUM8-1  
    C  
    C OBTAIN CORRECTIONS TO THE ESTIMATES  
    C  
      KK = L + 1  
      OLNT= X(I02)  
      IF (TP) OLNT=0.  
      DO 101 J=1,NS  
        IF (IUSEV(J)) I01=98,I00  
        9% DELN(J) = HQ(J)*OLNT-HC(J)+S(J)-ENLN(J)-TM*X(IG1)  
        DO 99 K=1,L  
          DELN(J)= DELN(J)+A(K,J)*X(K)  
        99 CONTINUE  
        GO TO 101  
180 100 DELN(J) = X(KK)  
      KK = KK + 1  
      101 CONTINUE  
      AMEDA= 1.  
      AMEDA1= 1.  
      SUP = X(I01)  
190 IF (SUM.LT.0.) SUM=SUM  
      IF (OLNT.GT.SUM) SUM=OLNT  
      IF (-OLNT.GT.SUM) SUM=-OLNT  
      DO 917 J=1,NS  
        IF (IUSEV(J).NE.0) GO TO 917  
        IF (EN(J,NPT).GT.0.) AND DELN(J).GT.SUM) SUM = DELN(J)  
        IF (TEP(NPT).NE.0.) OR DELN(J).LE.0.) GO TO 917  
        SUP1 = (-9.212-ENLN(J)+ENLN)/(DELN(J)-X(I01))  
        IF (SUM1.LT.0.) SUM1=-SUM1  
        IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1  
200 917 CONTINUE  
      IF (SUM.GT.2.) AMBDA=2./SUM  
      IF (AMBDA1.LT.AMBDA1) AMBDA = AMBDA1  
      IF (.NOT.IDE9UG) GO TO 111  
      WRITE(6,923) TT,ENN,ENLN,PP,PPLN,AMBDA  
205 923 FORMAT (3HJ1=E15.3,6H ENN=E15.3,7H ENLN=E15.3,5H PP=E15.3,  
        1 7H PPLN=E15.3,8H AMBDA=E15.3)  
      WRITE (6,924)  
210 924 FORMAT (10H 18X,2HNI,12X,2HNLN,18X,9HDEL LN NI,10X,4HMT,RT,9X,4HMS07  
        12X,6H-G0/RT,9X,5H-G/RT )  
      DO 926 J=1,NS  
        FNEG1 = S(J)-H0(J)  
        FNEG2 = FNEG1
```

215	IF (IUSE(J).EQ.0) FNEG2=FNEG2-ENLN(J)*TH WRITE (6,325) SUB(J,1),SUB(J,2), 1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),H3(J),S(J),FNEG1,FNEG2 925 FORMAT (1X,3A4,7E15.5) 926 CONTINUE WRITE (6,110) 110 FORMAT (1H0)	P1712 00885 P1712 00866 P1712 00867 P1712 00868 P1712 00869 P1712 00870 P1712 00871 P1712 00872 P1712 00873 P1712 00874 P1712 00875 P1712 00876 P1712 00877 P1712 00878 P1712 00879 P1712 00880 P1712 00881 P1712 00882 P1712 00883 P1712 00884 P1712 00885 P1712 00886 P1712 00887 P1712 00888 P1712 00889 P1712 00890 P1712 00891 P1712 00892 P1712 00893 P1712 00894 P1712 00895 P1712 00896 P1712 00897 P1712 00898 P1712 00900 P1712 00901 P1712 00902 P1712 00903 P1712 00904 P1712 00905 P1712 00906 P1712 00907 P1712 00908 P1712 00909 P1712 00910 P1712 00911 P1712 00912 P1712 00913 P1712 00914 P1712 00915 P1712 00916 P1712 00917
220	C C C 111 SUM = 0. DO 113 J=1,NS 112 ENLN(J)=ENLN(J)+AMBDA*DELN(J) EN(J,NPT) = 0. IF (ENLN(J)-ENLN+SIZE).LE.0.) GO TO 113 EN(J,NPT) = EXP(ENLN(J)) SUM = SUM+EN(J,NPT) GO TO 113	
225	114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J) 115 CONTINUE SUMN = SUM IF (TP) GO TO 115 TLN= TLN+AMBDA*DLNT TLN = EXP(TLN) 115 ENLN = ENLN+AMBDA*X(IG1) ENN = EXP(ENLN) IF (LLHT(L).NE.1E) GO TO 116	
235	C C C CHECK ON REMOVING IONS DO 1116 J = 1,NS IF (AL(J).EQ.0.) GO TO 1116 IF (EN(J,NPT).GT.0.) GO TO 116 1116 CONTINUE DO 1118 J=1,NS IF (AL(J).NE.0.) IUSE(J) = -10000 1118 CONTINUE L = L-1 IG1 = IG1-1 GO TO 43	
245	C C C TEST FOR CONVERGENCE 116 IF (ITNU*8.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 139 AA= DELN(J)/SUMN IF (AA.LT.0.) AA=-AA	
255		
260		
265		

```

129 IF (IUSE(J).EQ.0) XE = XEEN(J,NPT)
130 CONTINUE
131 CONVE = .TRUE.
270 IF (TT.LT.TLO..OR..TT.GT.THIGH..AND..IODEUG) WRITE(6,J36) TT,NPT
306 FORMAT(17H) THE TEMPERATURE=12.4,26H IS OUT OF RANGE FOR PCINT,15)
IF (TT.NGT.TNE..J) GO TO 167
WRITE(6,J37) TT,NPT
973 FORMAT(17H) 12,59H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIRE
METS FOR THE POINT 15)
IF (.NOT..HP..OR..APY..NE..1..OR..NC.EQ..0..OR..TT.GT.100.) GO TO 873
WRITE(6,J38)
TT = TTII
RETURN
280 C
281 C CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.
282 C
160 IF (NC.EC.G) GO TO 143
SIZE = 0
INC = 0
DO 170 J = 1,NS
IF (IUSE(J).EC.0 .OR. IUSE(J).EQ.-10000) GO TO 170
INC = INC + 1
IF (IODEUG) WRITE(6,144)(SU3(J,I),I=1,3),TEMP(INC,2),TEMP(INC,2)
IUSE(J) = 0
144 FORMAT (10H,144,2F10.3,3X,5H) IUSE=,14,215.7)
IF (IEN(J,NPT)) 146,146,159
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 KC = 1
IF (IUSE(J).EQ.-IUSE(J+1)) GO TO 154
IF (J.EC.1..OR..IUSE(J).NE.-IUSE(J-1)) GO TO 153
KC = -1
154 JAG = J + KC
IF (CENTXG,NPT).LT.0.) GO TO 170
TKELT = TEMP(INC,1)
TMP = INC + KC
IF (TKELT.EQ.TEMP(IMP,2)) GO TO 154
TKELT = TEMP(IMP,2)
IF (TKELT.EQ.TEMP(IMP,1)) GO TO 157
WRITE (6,156)
156 FORMAT (50H) 3 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER )
C
C JTM SPECIES A SOLID (EN=0), (J+KC)TH SPECIES A LIQUID (EN IS +)
C
157 IF (TT.GT.TMELT) GO TO 169
IF (P..AND..TT.EQ.TMELT) GO TO 165
IF (TP) GO TO 1165
IF (TT.LE.TMELT-150.) GO TO 1165

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```

320      JSQ = J
      JLIQ = JKG
      GO TO 159

      C
      C JTH SPECIES A LIQUID(EN=0), (J*KG)TH SPECIES A SOLID (EN IS +)
      C
325      IF (TT.LT.TMELT) GO TO 169
      IF (TP.AND.TT.EQ.TMELT) GO TO 169
      IF (TP) GO TO 1165
      IF (TT.GE.TMELT+150.) GO TO 1165
      JSOL = JKG
      JLIQ = J
330      TTN = ALOG(TMELT)
      TT = TMELT
      EN(JKG,NPT) = .5 * EN(JKG,NPT)
      EN(J,NPT) = EN(JKG,NPT)
      GO TO 165

335      C
      C WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN
      C
340      1165 EN(J,NPT) = EN(JKG,NPT)
      IUSE(J) = -IUSE(J)
      IUSE(JKG) = -IUSE(JKG)
      EN(JKG,NPT) = 0.
      GO TO 160

345      153 IF (TT.LT.TEMP(INC,1) .AND. TEMP(INC,1) .NE. TLON) GO TO 169
      IF (TT.GT.TEMP(INC,2)) GO TO 169

      C
      C
      SUM = 0.
      DO 167 I = 1, L
      SUM = SUM + A(I,J)*X(I)
350      167 CONTINUE
      DELF = H1(J)-S(J)-SUM
      IF (IDEBUG) WRITE(6,168) DELF, SIZEF
      168 FORMAT (17H GO-SUM(AIJ*PI) = E15.7, 10X, 18HPREVIOUS DELTA S = E15.7)
      IF (DELF.GE.SIZEF) FORK = DELF.GE.0. GO TO 169
      SIZEF = DELF
      JOELF = J
355      169 IF (INC.EQ.NC) GO TO 1160
      170 CONTINUE
      1160 IF (SIZEF.EQ.0.) GO TO 143
      J = JOELF

360      165 IC1 = IC1 + 1
      166 IUSE(J) = - IUSE(J)
      167 CONVG = .FALSE.
      163 TN = NUM9
      IF (IDEBUG) WRITE(6,771) NPT, (X(IIL), IL=1,L), TN
      771 FORMAT (13,14F9.3)
      ITNUM9 = ITN
      GO TO 143

370      C
      C CALCULATE EQUILIBRIUM PROPERTIES

```

P1712 00971
P1712 00972
P1712 00973
P1712 00974
P1712 00975
P1712 00976
P1712 00977
P1712 00978
P1712 00979
P1712 00980
P1712 00981
P1712 00982
P1712 00983
P1712 00984
P1712 00985
P1712 00986
P1712 00987
P1712 00988
P1712 00989
P1712 00990
P1712 00991
P1712 00992
P1712 00993
P1712 00994
P1712 00995
P1712 00996
P1712 00997
P1712 00998
P1712 00999
P1712 01000
P1712 01001
P1712 01002
P1712 01003
P1712 01004
P1712 01005
P1712 01006
P1712 01007
P1712 01008
P1712 01009
P1712 01010
P1712 01011
P1712 01012
P1712 01013
P1712 01014
P1712 01015
P1712 01016
P1712 01017
P1712 01018
P1712 01019
P1712 01020
P1712 01021
P1712 01022
P1712 01023

171	SSUM(NPT) = 0.	P1712	01024
	IF(JLID,NE,0) EN(JSOL,NPT)=ENSOL	P1712	01025
375	DO 183 J=1,NS	P1712	01026
	IF (NPT,EG,1) SS0 = SS0 + EN(J,1)*S(J)	P1712	01027
	SS = S(J)	P1712	01028
	IF(IUSEVJT,EG,UJ) SS=SS-EN(N(J),TJ)	P1712	01029
	SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)	P1712	01030
380	CONTINUE	P1712	01031
	IF(.NOT.IC) GO TO 176	P1712	01032
	GLVPT(NPT) = -1.	P1712	01033
	DLVPT(NPT) = 1.	P1712	01034
	CPR(NPT) = CPSSUM	P1712	01035
385	GO TO 199	P1712	01036
	SUM = 0.	P1712	01037
178	DO 179 J = 1,L	P1712	01038
	SUM = SUM + PROK(J)*X(J)	P1712	01039
179	CONTINUE	P1712	01040
	DLVPT(NPT) = -2.*SUM/ENN*X(IQ1)	P1712	01041
390	IF(JLIC,EG,0) GO TO 199	P1712	01042
	IUSE(JLIC) = -IUSE(JLIC)	P1712	01043
	HSUM(NPT) = HSUM(NPT)+EN(JLIC,NPT)*(H0(JLIC)-H0(JSOL))	P1712	01044
	IQ1 = IQ1+1	P1712	01045
395	GAMMAS(NPT) = -1./DLVPT(NPT)	P1712	01046
	GO TO 185	P1712	01047
	199 GAMMAS(NPT) = -1./ (DLVPT(NPT) + (DLVPT(NPT)**2)*ENN/CPR(NPT))	P1712	01048
50	ITT(NPT) = TT	P1712	01049
	PP(NPT) = PP	P1712	01050
400	CPR(NPT) = CPSSUM	P1712	01051
	HSUM(NPT) = HSUM(NPT)*TT	P1712	01052
	MM(NPT) = 1./ENN	P1712	01053
	IF (.NOT.IDEBUG) RETURN	P1712	01054
405	WRITE(6,201) NPT,PCPINPT),PP,TT,HSUM(NPT),SSUM(NPT),MM(NPT),CPR(NPT)	P1712	01055
	17).DLVPT(NPT),DLVPT(NPT),GAMMAS(NPT)	P1712	01056
201	FORMAT (7HOPINT=I3,X,4HPCP=E13.6,X,2HP=E13.6,X,2HT=E13.6,X,4H	P1712	01057
	1H/R=E13.6,X,4HHS/R=E13.6/X,3HMM=E13.6,X,5HCP/R=E13.6,X,6HDLVPT	P1712	01058
	2=E13.6,X,6HDLVPT=E13.6,X,9MGAMMA(S)=E13.6)	P1712	01059
	GO TO 1000	P1712	01060
410	C	P1712	01061
	C	P1712	01062
	C	P1712	01063
873	TT=0.	P1712	01064
	NPT = NPT+1	P1712	01065
415	1000 RETURN	P1712	01066
	END	P1712	01067
		P1712	01068

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PAGE NO. 1

SUBROUTINE FROZEN

C

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05

{FROZEN COMPOSITION EXPANSION ONLY}

LOGICAL EQL,FROZ,CONVG

10

```
COMMON/POINTS/RSUM(13),SSUN(13),CPR(13),OLVTP(13),OLVPT(13)
1  GAMMAS(13),PIZ(26),Y(26),V(13),PPF(13),WM(13),SONVEL(13),YTT(13)
2  TCTN(13)
COMMON/SPECIES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),H0(150)
1  DELN(150),A(15,150),SUB(150,3),IUSE(150),TEMP(50,2)
```

15

```
COMMON/RTSC/ENN,SUMN,TT,SH,ATGR(13,101),LLRT(15),BU(15,2)
1  TM,TLCH,TMIO,THIGH,PF,SH,UN,OF,EORAT,FPCT,R,RR,HSUB90,AC(2),AM(2)
2  HPP(2),RHO(2),VMIN(2),LS(2),MP(2),DATA(22),NAME(15,5)
3  ANUM(15,5),PECHT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)
4  RHOP,RHM(15),TLN,JANF
```

20

```
COMMON/INDEX/IOEBUG,CONVG,IP,HP,SP,HPSP,TPSP,MOLES,MP,NT,NPT,L,NS,
1  KHAT,INAT,TOL,N,J,NOMIT,IP,NEWK,NSUB,NSUP,ITR,GPCVFR,CPCEVO
2  IONS,AC,NSERT,JSOL,JLIO,KASE(14),NREAC,IC,IQ2
COMMON/PERF/PCP(26),VMOC(13),SPIN(13),VAGI(13),SUBAR(13),SUPAR(13)
```

25

```
1  CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO
COMMON/OUP/FT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)
1  FG(4),FG(4),FB,FHT13,F1,F2,F3,F4,F5,FL(4),FMT19,FA1,FA2
2  FRI,FCI,FN(4),F(4),FA(4),FI(4),FMT9X,FO
```

30

```
ITROT = 3
EQL = .FALSE.
NPT = 2
TT = TTT(1)
TLN=ALOG(TT)
```

35

```
GAMMAS(I) = CPRF(I)/CPRF(I)*1.7MN(1)
CPR(1) = CPRF(1)
PCP(2) = ((GAMMAS(1)+1.)/2.)*((GAMMAS(1)/(GAMMAS(1)-1.))
DATA(1) = 2./(GAMMAS(1) + 1.)
TLN = TLN + ALOG(DATA(1))
DO 902 IP=2,NP
```

40

```
IF(NPT.EQ.2) GO TO 45
PCP(NPT) = P(1)/P(IP)
CONVG = .FALSE.
PCPLH=ALOG(PCP(NPT))
S0 = SSO -PCPLN/NM(1)
SUMH = 0.
```

45

```
51 TT=EXP(TENT)
SUNS=0.
J = 1
NNA = NPT
NPT = 1
CALL GPHS
NPT = NM
```

50

```
DO 60 J=1,NS
IF(EN(J,1).EQ.0.) GO TO 63
SUMS = SUMS + S(J)*EN(J,1)
IF(CONVG) SUMH=SUMH+H0(J)*EN(J,1)
```

55	60 CONTINUE	P1712 01122
	IF (CONVG) GO TO 81	P1712 01123
	ULNT=(SUMS-50)/CPSUM	P1712 01124
	TUA=TLN-DLNT	P1712 01125
	IF (DLNT.LT.0.) DLNT=-DLNT	P1712 01126
	IF (DLNT.LT.U.5E-4) CONVG=.TRUE.	P1712 01127
60	GO TO 51	P1712 01128
	81 ITI(NPT)= IT	P1712 01129
	SSUM(NPT)= SSUM(1)	P1712 01130
	HSUM(NPT)= IT*SUM	P1712 01131
	GAMMAS(NPT)= CPSUM/(CPSUM-1./NM(1))	P1712 01132
65	IF (IP.GT.2) GO TO 90	P1712 01133
	GO TO 51	P1712 01134
	C	P1712 01135
	C	P1712 01136
	C	P1712 01137
70	OH = HSUM(1)-HSUM(2)	P1712 01138
	OHSTAR = OH-(GAMMAS(2)*TT/(2.*NM(1)))	P1712 01139
	OH = OHSTAR/OH	P1712 01140
	IF (OH.LT.0.) OH=-OH	P1712 01141
	IF (OH.L. 0.4E-4.OR. ITROT.EQ.0) GO TO 90	P1712 01142
75	PCP(2) = PCP(2)/(1.+2.*OHSTAR*NM(1)/(IT*(GAMMAS(2)+1.)))	P1712 01143
	P(2) = P(1)/PCP(2)	P1712 01144
	ITROT = ITROT-1	P1712 01145
	GO TO 45	P1712 01146
	90 NP(NPT)= NM(1)	P1712 01147
80	PP(NPT) = P(IP)	P1712 01148
	CP(NPT)= CPSUM	P1712 01149
	K = 0	P1712 01150
	IF (TT.LT.(TLOW-150.)) GO TO 903	P1712 01151
	IF (NC.EQ.0) GO TO 700	P1712 01152
	INC = 1	P1712 01153
85	DO 901 I=1,NS	P1712 01154
	IF (IUSE(I).EQ.0.OR.IUSE(I).EQ.-10000) GO TO 901	P1712 01155
	INC = INC+1	P1712 01156
	IF (EM(I).EQ.0.) GO TO 901	P1712 01157
	IF (TT.LT.(TEMP(INC)-50.))OR.TT.GT.(TEMP(1)+50.))GO TO 903	P1712 01158
90	901 CONTINUE	P1712 01159
	700 IF (IP.EQ.NP) GO TO 863	P1712 01160
	K = NPT	P1712 01161
	IF (NPT.NE.13) GO TO 870	P1712 01162
	GO TO 863	P1712 01163
95	903 NP1 = NPT - 1	P1712 01164
	863 CALL RKROUT	P1712 01165
	IF (NSUB+NSUP.NE.0) CALL RATIO	P1712 01166
	865 IF (K.EQ.0) GO TO 1002	P1712 01167
	NPT = 2	P1712 01168
100	870 NPT = NPT + 1	P1712 01169
	902 CONTINUE	P1712 01170
	1000 RETURN	P1712 01171
	END	

05	C	SUBROUTINE HCALC	P1712 01172
	C	CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS	P1712 01173
	C		P1712 01174
	C		P1712 01175
	C		P1712 01176
	C		P1712 01177
	C	LOGICAL MOLES	P1712 01178
	C	DIMENSION NUM(15),S(2),WS(2)	P1712 01179
10	C	COMMON/SPACES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),M0(150)	P1712 01180
	C	1,DELN(150),A(15,153),SUB(150,3),IUSE(150),TEMP(50,2)	P1712 01181
	C	COMMON/MISC/ENR,SUMN,IT,S0,ATOM(1,101),LLMT(15),30(15),80P(15,2)	P1712 01182
	C	1,FM,7LCM,THIO,THIGH,PP,CPSUM,OF,EGRAT,FPST,R,RR,MSUB0,AC(2),AM(2)	P1712 01183
	C	2,HP(12),RHO(12),VMIN(2),VPLS(12),MP(2),DATA(22),NAME(15,5)	P1712 01184
	C	3,ANUM(15,5),PECHT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)	P1712 01185
	C	4,RHOP,RHM(15),TLN,JANF	P1712 01186
15	C	COMMON/INCH/ IDEBUG,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,	P1712 01187
	C	1,KHAT,IMAT,IQI,N,J,NOMIT,IP,NEWQ,NSUB,NSUP,IIN,CPCVFR,CPCVED	P1712 01188
	C	2,IONS,NC,INSERT,JSOL,JLIQ,KASE(14),NREAC,IC,IQ2	P1712 01189
20	C	EQUIVALENCE(ANUM,NUM)	P1712 01190
	C		P1712 01191
	C		P1712 01192
	C	DATA AG/1HG/,IZERO/2H00/,OX/1H0/	P1712 01193
25	C	IS IT IN RANGE	P1712 01194
	C		P1712 01195
	C		P1712 01196
	C	IF(IT.LI.(TLOW-100.).OR.IT.GT.(THIGH+1000.))GO TO 80	P1712 01197
	C	WS(1) = 0.	P1712 01198
	C	WS(2) = 0.	P1712 01199
	C	HP(1) = 0.	P1712 01200
	C	HP(2) = 0.	P1712 01201
30	C	AC(1) = 0.	P1712 01202
	C	AC(2) = 0.	P1712 01203
	C	DO 900 N=1,NREAC	P1712 01204
	C	K=2	P1712 01205
35	C	IF(FOX(N).EQ.OX)K=1	P1712 01206
	C	PCNT=PECHT(N)	P1712 01207
	C	IF(THOLES)PCNT=PCNT+RHM(N)	P1712 01208
	C	WS(K) = WS(K) + PCNT	P1712 01209
	C	J = NUM(N,5)	P1712 01210
40	C	IF (J.NE.3) GO TO 90	P1712 01211
	C	DO 11 J=1,L	P1712 01212
	C	DATA(J)=0.	P1712 01213
	C	10 CONTINUE	P1712 01214
	C	DO 40 I=1,4	P1712 01215
45	C	IF(ANUM(N,I).EQ.0.)GO TO 50	P1712 01216
	C	DO 20 J=1,L	P1712 01217
	C	IF(ILLMT(J).EQ.NAME(N,I)) GO TO 30	P1712 01218
	C	20 CONTINUE	P1712 01219
	C	30 DATA(J)=ANUM(N,I)	P1712 01220
50	C	40 CONTINUE	P1712 01221
	C	50 IS=0	P1712 01222
	C	DO 70 J=1,NS	P1712 01223
	C	IF(IUSE(J).EQ.0)GO TO 55	P1712 01224

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55      IS = IS+1
      IF (FAZ(N).EQ.AG) GO TO 70
      IF (IT.LY.TEMP(IS,1).OR.IT.JT.TEMP(IS,2)) GO TO 70
      GO TO 56
56      IF (FAZ(N).EQ.AG) GO TO 70
56      DO 60 I=1,L
      IF (ATIT,JT.NE.DATA(IT)) GO TO 70
      60 CONTINUE
      NUM(N,5) = J
      GO TO 90
      70 CONTINUE
      GO TO 80
56      NSS = NS
      NS = J
      CALL CP+S
      GPSUM = GPSUM/EN(J,HPT)
      NS = NSS
      IF (H0(J).GT.-.01 .AND. H0(J).LT..01) H0(J) = 0.
      RTEMP(N) = IT
      ENTH(N) = HU(J)*RT
      AC(N) = AC(K)+GPSUM*PCHT/RMW(N)
      HPP(K) = HPP(K)+ENTH(N)*PCWT/RMW(N)
      500 CONTINUE
      DO 950 K=1,2
      IF (HPT(K).EQ.0) GO TO 950
      HPP(K) = HPP(K)/WS(K)
      AC(K) = AC(K)/WS(K)
      950 CONTINUE
      HSUBJ = (HP(1)*HPP(1)+HP(2)*HPP(2))/(HP(1)+HP(2))
      GO TO 1000
      80 WRITE(5,95) N
      85 FORMAT(1H0,12,34HITH REACTANT IS NOT IN THERMO DATA )
      1300 RETURN
      END

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P1712 01225
 P1712 01226
 P1712 01227
 P1712 01228
 P1712 01229
 P1712 01230
 P1712 01231
 P1712 01232
 P1712 01233
 P1712 01234
 P1712 01235
 P1712 01236
 P1712 01237
 P1712 01238
 P1712 01239
 P1712 01240
 P1712 01241
 P1712 01242
 P1712 01243
 P1712 01244
 P1712 01245
 P1712 01246
 P1712 01247
 P1712 01248
 P1712 01249
 P1712 01250
 P1712 01251
 P1712 01252
 P1712 01253
 P1712 01254
 P1712 01255
 P1712 01256
 P1712 01257
 P1712 01258

Line	Code	Statement	Labels
05	C	SUBROUTINE MATRIX	
	C	DOUBLE PRECISION G,X	
	C	LOGICAL HP,SP,IF,IOEBUG,CONVG,NEWK	
10	C	COMMON/POINTS/HSUB(13),SSUM(13),CPR(13),DELVTP(13),ULVPT(13), 1 GANVPS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TIT(13), 2 TCTN(13)	P1712 01259 P1712 01260 P1712 01261 P1712 01262 P1712 01263 P1712 01264 P1712 01265 P1712 01266 P1712 01267 P1712 01268 P1712 01269 P1712 01270 P1712 01271 P1712 01272 P1712 01273 P1712 01274 P1712 01275 P1712 01276 P1712 01277 P1712 01278 P1712 01279 P1712 01280 P1712 01281 P1712 01282 P1712 01283 P1712 01284 P1712 01285 P1712 01291 P1712 01292 P1712 01293 P1712 01294 P1712 01299 P1712 01296 P1712 01297 P1712 01298 P1712 01299 P1712 01300 P1712 01302 P1712 01303 P1712 01304 P1712 01305 P1712 01306 P1712 01307 P1712 01308 P1712 01309 P1712 01310 P1712 01311
15	C	COMMON/SPECES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),MO(150), 1 BELN(15),A(15,150),SUB(15,3),IUSE(150),TEMP(50,2) COMMON/MISC/ENN,SUMN,IT,SU,ATON(3,10),LLMT(15),BO(15),BOP(15,2) 1 TM,TLCK,TMID,THIGH,PF,CPSUM,OF,EQRT,FPST,R,WR,HSUB0,ACT2),AM(2) 2 PPR(2),PHO(2),VMIN(2),VPLS(2),MP(2),DATA(22),NAME(15,5) 3 ANUM(15),PECDT(15),ENTH(15),FAZ(15),RIEMP(15),FOX(15),DENS(15) 4 RHOP,RMH(15),TLN,JANF COMMON/DOUBLE/ G(20,21), X(20) COMMON/INDEX/ IOEBUG,CONVG,TP,HP,SP,MPSP,TPSP,MOLES,NP,MT,HP,T,L,NS, 1 KMAT,IVAT,IOI,N:J,NOMIT,IP,NEWK,NSUB,NSUP,ITN,CPGVR,CPCTVEG 2 IONS,AC,NSERT,JSOL,JLJO,KASE(14),NREAC,IC,IO2 IO2 = IO1 + 1 IO3 = IO2 + 1 KMAT = IO3 IF(.NOT.CONVG.AND.TP) KMAT = IO2 IMAT = PHAT - 1	
20	C	CLEAR MATRIX STORAGES TO ZERO	
25	C	DO 211 I=1,IMAT DO 211 K=1,KMAT G(I,K) = 0.000 G(I,K) = 0.0 211 CONTINUE SSS = 0. HSCUM(NPT) = 0.	
30	C	BEGIN SET UP OF ITERATION MATRIX	
35	C	KK = L DO 65 J=1,NS H=H0(J)*EN(J,NPT) IF (IUSE(J)) 65,11,70 11 F = (H0(J)-S(J)+ENLN(J)+IN)*EN(J,NPT) SS = M-F TERM1 = H IF (KMAT.EQ. IO2) TERM1 = F DO 55 I = 1, L	
40	C	CALCULATE THE ELEMENTS R(I,K)	
45	C	IF (A(I,J).EQ. 0.) GO TO 55 TERM = A(I,J)*EN(J,NPT)	
50	C		

55	DC 15 K=1, C	P1712 01312
	G(I,K) = G(I,K) + A(I,J)*TERM	P1712 01313
	15 CONTINUE	P1712 01314
	C	P1712 01315
	G(I,IQ1)=G(I,IQ1)+TERM	P1712 01316
60	G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1	P1712 01317
	IF (CONVG=.OR.1) 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
65	IF (KNAT .EQ. IC2) 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)+H0(J)*SS	P1712 01325
	G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - EMLN(J)-TM)*F	P1712 01326
	GO TO 62	P1712 01327
70	59 G(IQ2,IQ2)=G(IQ2,IQ2)+H0(J)*H	P1712 01328
	IF (CONVG) GO TO 64	P1712 01329
	G(IQ2,IQ3)=G(IQ2,IQ3)+H0(J)*F	P1712 01330
	62 G(IQ1,IQ3)=G(IQ1,IQ3)+F	P1712 01331
75	64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM	P1712 01332
	GO TO 65	P1712 01333
	C	P1712 01334
	C CONDENSED SPECIES	P1712 01335
	70 KK = KK + 1	P1712 01336
80	00 75 I = 1, L	P1712 01337
	G(I,KK) = A(I,J)	P1712 01338
2	G(I,KK) = G(I,KK) - A(I,J)*EN(J,NPT)	P1712 01339
	75 CONTINUE	P1712 01340
	G(KK,IQ2) = H0(J)	P1712 01341
85	G(KK,KK) = H0(J) - S(J)	P1712 01342
	MSUM(NPT) = MSUM(NPT) + M	P1712 01343
	IF (.NOT.SP) GO TO 55	P1712 01344
	SSS = SSS + S(J)*EN(J,NPT)	P1712 01345
	G(IQ2,KK) = S(J)	P1712 01346
90	65 CONTINUE	P1712 01347
	SSS = SSS + G(IQ2,IQ1)	P1712 01348
	MSUM(NPT) = MSUM(NPT) + G(IQ1,IQ2)	P1712 01349
	G(IQ1,IQ1) = SUMN - ENN	P1712 01350
95	C	P1712 01351
	C REFLECT SYMMETRIC PORTIONS OF THE MATRIX	P1712 01352
	ISYM = IQ1	P1712 01353
	IF (HP.OR.CONVG) ISYM=IQ2	P1712 01354
100	00 102 I=1, ISYM	P1712 01355
	00 102 J=I, ISYM	P1712 01356
	G(J,I)=G(I,J)	P1712 01357
	102 CONTINUE	P1712 01358
	C	P1712 01359
	C COMPLETE THE RIGHT HAND SIDE	P1712 01360
105	C	P1712 01361
	IF (CONVG) GO TO 175	P1712 01362
		P1712 01363
		P1712 01364

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110      DC 145 I=1,L
          X(I)=30(I)-G(I,IQ1)
          G(I,KMAT) = G(I,KMAT)+X(I)
          145 CONTINUE
          G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN
          C
          C COMPLETE ENERGY ROW AND TEMPERATURE COLUMN
          C
          IF (KMAT.EQ. IC2) GO TO 105
          IF (SP)ENERGY = S0+ENN-SUMN - SSS
          IF (HP)ENERGY=HSUR0/TT - HSUM(NPT)
          G(IQ2,IC3)=G(IQ2,IC3)+ ENERGY
          175 G(IQ2,IC2)=G(IC2,IC2)+CPSUM
          105 RETURN
          ENC
120

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P1712 01365
 P1712 01366
 P1712 01367
 P1712 01368
 P1712 01369
 P1712 01370
 P1712 01371
 P1712 01372
 P1712 01373
 P1712 01374
 P1712 01375
 P1712 01376
 P1712 01377
 P1712 01378
 P1712 01379


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55      28 IF (NN-I) 29,31,29
      29 DO 30 J=NN,IUSE1
      30 Z=G(I,J)
      31 G(I,J)=G(NN,J)
      32 G(NN,J)=Z
      33 CONTINUE
      34 DIVIDE A11 ROW BY A11 DIAGONAL ELEMENT AND ELIMINATE THE NTH
      35 VARIABLE FROM THE REMAINING EQUATIONS
      36 K = NN + 1
      37 DO 38 J = K, IUSE1
      38 IF (G(NN,J) .EQ. 0.) GO TO 23
      39 G(NN,J) = G(NN,J) / G(NN,NN)
      40 CONTINUE
      41 IF (K-IUSE1) 46,45,38
      42 DO 44 I = K, IUSE1
      43 DO 44 J = K, IUSE1
      44 G(I,J) = G(I,J) - G(I,NN)*G(NN,J)
      45 CONTINUE
      46 BACKSOLVE FOR THE VARIABLES
      47 K = IUSE1
      48 J = K + 1
      49 X(K) = 0.000
      50 X(K) = 0.3
      51 SUM = 0.0
      52 IF (IUSE1 - J) 51,49,48
      53 DO 54 I = J, IUSE1
      54 SUM = SUM + G(K,I) * X(I)
      55 CONTINUE
      56 X(K) = G(K,IUSE1) - SUM
      57 K = K - 1
      58 IF (K) 67,151,57
      59 IUSE1 = IUSE1 - 1
      60 RETURN
      61 END

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P1712 01438
 P1712 01439
 P1712 01440
 P1712 01441
 P1712 01442
 P1712 01443
 P1712 01444
 P1712 01445
 P1712 01446
 P1712 01447
 P1712 01448
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 P1712 01450
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 P1712 01460
 P1712 01461
 P1712 01462
 P1712 01463
 P1712 01464
 P1712 01465
 P1712 01466
 P1712 01467
 P1712 01468
 P1712 01469
 P1712 01470
 P1712 01471

05	C	SUBROUTINE MOLIER	P1712 01472
		COMMON/POINTS/MSUM(13),SSUM(13),CPR(13),OLVFP(13),JLVFP(13)	P1712 01473
		1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),MM(13),SONVEL(13),TTT(13)	P1712 01474
		2 ,TCFN(13)	P1712 01475
		COMMON/SPECIES/DOEF(2,7,150),S(150),EN(150,13),EALN(150),MO(150)	P1712 01476
		1 ,TENT(150),A(15,150),SU(150,3),IUSE(150),TEMP(150,2)	P1712 01477
		COMMON/MISC/ERN,SUMM,II,SU,ATOM(13,10),LLM(15),BU(15),BDP(15,2)	P1712 01478
		1 ,TK,TLOM,THIO,THIGH,PP,CPSUM,OF,EGRAI,FPC,R,R,MSUBO,AC(2),AM(2)	P1712 01479
		2 ,MP(12),AMO(12),VMI(12),VPLS(12),MP(12),DATA(22),NAME(15,5)	P1712 01480
		3 ,ANUM(15,5),PCMF(15),ENT(15),FAZ(15),RTCMP(15),FOX(15),DEMS(15)	P1712 01481
		4 ,RHOP,R4M(15),ILN,JANF	P1712 01482
		COMMON/INDEX/IDCRUG,CONVG,IP,NP,SP,NDSF,TPSP,MOLES,NP,NT,L,NS,	P1712 01483
		1 ,KHA7,I7AT,I3I,N,J,NOMIT,IP,NEWZ,NSUB,ASUP,ITN,OPCVFR,CPCVE3	P1712 01484
		2 ,IONS,NC,INSERT,J,SOL,JULIQ,KA5E(14),NREAC,IC,JO2	P1712 01485
		DO 91 IT = 1,26	P1712 01486
		IF (IT) EQ. 0.7 GO TO 95	P1712 01487
		NT = IT	P1712 01488
		91 CONTINUE	P1712 01489
20	C	SET ASSIGNED P	P1712 01490
	C	92 DO 902 IP = 1,NP	P1712 01491
		PP = P(IP)	P1712 01492
	C	SET ASSIGNED :	P1712 01493
	C	DO 902 I3=1,NT	P1712 01494
		IT = (IT)	P1712 01495
		CALL EQLDRM	P1712 01496
30		IF (IT) EQ. 0 GO TO 302	P1712 01497
		IF (NP) EQ. 1 GO TO 1000	P1712 01498
		IF (IP) EQ. 0 GO TO 860	P1712 01499
		K = NP	P1712 01500
		IF (NP) EQ. 1 GO TO 870	P1712 01501
35		5 FORMAT(1M1,41X,6HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED	P1712 01502
		1 ,/43X,28H TEMPERATURES AND PRESSURES ///	P1712 01503
		CALL OUT1	P1712 01504
		WRITE (6,863)	P1712 01505
		FORMAT (25HTHERMODYNAMIC PROPERTIES//)	P1712 01506
		CALL OUT2	P1712 01507
		CALL OUT3	P1712 01508
45		865 IF (K) EQ. 0 GO TO 1000	P1712 01509
		WRITE (6,866)	P1712 01510
		56A FORMAT(1M1)	P1712 01511
		NP = 0	P1712 01512
		970 NP = NP + 1	P1712 01513
		971 NP = NP + 1	P1712 01514
		CALL OUT3	P1712 01515
		WRITE (6,868)	P1712 01516
		56A FORMAT(1M1)	P1712 01517
		NP = 0	P1712 01518
		970 NP = NP + 1	P1712 01519
		971 NP = NP + 1	P1712 01520
50	C	SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT	P1712 01521
	C	DO 880 I = 1,NS	P1712 01522
		880 I = 1,NS	P1712 01523
		880 I = 1,NS	P1712 01524

08.09.56.

31/12/70

FORTAN EXTENDED VERSION 2.0

SUBROUTINE HOLIER

EN(I,NFY) = EN(I,K)

880 CONTINUE

962 CONTINUE

1000 RETURN

END

P1712 01525
P1712 01526
P1712 01527
P1712 01528
P1712 01529

08.09.56.

31/12/70

FORTAN EXTENDED VERSION 2.0

SUBROUTINE OUT1

```

55      HD1 = C*10
      HD2 = ANT
      GO TO 11
      10 HD1 = FUEL
      HD2 = FB
      11 DO 13 J=1,5
      13 CONTINUE
      14 J=J-1
      HD3(3)=YN(J)
      HD3(7)=YX(J)
      WRITE(6,HEAD)HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ,PECHT(N),ENTHT
      1N),FAZ(N),RTMP(N),DENS(N)
      15 CONTINUE
      WRITE(6,20) OF,FCPT,EGRAT,RHOP
      20 FORMAT (1H0,15X, 4H0/F=, F8.4,4X,13HPERCENT FUEL=,F8.4,4X,
      1 19HEQUIVALENCE RATIO=,F7.4,4X,8HDENSITY=,F8.4//)
      C
      AGV = 9.80665
      DO 25 I = 1,NPT
      TOTN(I) = 0
      DO 25 J = 1,MS
      TOTN(I) = TOTN(I) + EN(J,I)
      25 CONTINUE
      FMT(4) = FMT(6)
      RETURN
      C
      ENTRY OUT2
      C
      C---PRESSURE
      C
      DO 55 I=1,NPT
      K= 2*I+3
      FMT(K) = F4
      IF (PPP(I).GE.1.) FMT(K)=F3
      IF (PPP(I).GE.10.) FMT(K)=F2
      IF (PPP(I).GE.100.) FMT(K)=F1
      55 CONTINUE
      WRITE (6,FMT) (FP(I),I=1,4), (PPR(J),J=1,NPT)
      C
      C---TEMPERATURE
      C
      DO 65 I=1,NPT
      NV(I) = TTI(I)*.5
      65 CONTINUE
      FMT(4) = FMT13
      FMT(5) = FMT19
      WRITE (6,FMT) (FI(I),I=1,4), (NV(J),J=1,NPT)
      C
      C---ENTHALPY
      C
      DO 75 I=1,NPT

```

P1712 01582
 P1712 01583
 P1712 01584
 P1712 01585
 P1712 01586
 P1712 01587
 P1712 01588
 P1712 01589
 P1712 01590
 P1712 01591
 P1712 01592
 P1712 01593
 P1712 01594
 P1712 01595
 P1712 01596
 P1712 01597
 P1712 01598
 P1712 01599
 P1712 01600
 P1712 01601
 P1712 01602
 P1712 01603
 P1712 01604
 P1712 01605
 P1712 01606
 P1712 01607
 P1712 01608
 P1712 01609
 P1712 01610
 P1712 01611
 P1712 01612
 P1712 01613
 P1712 01614
 P1712 01615
 P1712 01616
 P1712 01617
 P1712 01618
 P1712 01619
 P1712 01620
 P1712 01621
 P1712 01622
 P1712 01623
 P1712 01624
 P1712 01625
 P1712 01626
 P1712 01627
 P1712 01628
 P1712 01629
 P1712 01630
 P1712 01631
 P1712 01632
 P1712 01633
 P1712 01634

```

      V(I) = HSUM(I) * R
      75 CONTINUE
      FMT(5) = F9
      FMT(7) = F1
      WRITE (6,FMT) (FM(I), I=1,4), (V(J), J=1,NPT)
      C
      C ENTROPY
      C
      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) (FO(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) (FG(I), I=1,4), (VT(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) = SORT(R3 * GAMMAS(I) * TTT(I) / WM(I))
      95 CONTINUE
      WRITE (6,FMT) (FL(I), I=1,4), (SONVEL(J), J=1,NPT)
      VOLUME = GAMMAS(1) * TTT(1)
      IMPETUS = VOLUME * 2781. / WM(1)
      RETURN
      C

```

P1712 01635
 P1712 01636
 P1712 01637
 P1712 01638
 P1712 01639
 P1712 01640
 P1712 01641
 P1712 01642
 P1712 01643
 P1712 01644
 P1712 01645
 P1712 01646
 P1712 01647
 P1712 01648
 P1712 01649
 P1712 01650
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 P1712 01670
 P1712 01671
 P1712 01672
 P1712 01673
 P1712 01674
 P1712 01675
 P1712 01676
 P1712 01677
 P1712 01678
 P1712 01679
 P1712 01680
 P1712 01681
 P1712 01682
 P1712 01683
 P1712 01684
 P1712 01685
 P1712 01686
 P1712 01687

```

160  ENTRY OUT1
    IF (.NOT.EOL) GO TO 331
    C  MOLE FRACTIONS - EQUILIBRIUM
    C
165  WRITE (6,80)
    PRINT*,F5
    WRITE(6,310)
    310 FORMAT(15HMOLE FRACTIONS //)
    DO 330 K=1,NS
    330 K=1,NS
    DO 315 I=1,NPT
    315 I=1,NPT
    V(I) = EN(K,I) /TOTN(I)
    319 CONTINUE
    DO 316 I=1,NPT
    316 I=1,NPT
    IF (V(I).GE.(5.E-6)) GO TO 320
    320 CONTINUE
    320 WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT)
    321 CONTINUE
    331 WRITE(6,335)
    335 FORMAT(11SHADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MO
    1LE FRACTIONS WERE LESS THAN .00005 FOR ALL ASSIGNED CONDITIONS//)
    LINE= 0
    DO 340 K=1,NS
    340 K=1,NS
    IF ((EN(K,1)/TOTN(1)).GE.(5.E-6)) GO TO 343
    341 CONTINUE
    LINE= LINE+1
    Z(LINE,1) = SUB(K,1)
    Z(LINE,2) = SUB(K,2)
    Z(LINE,3) = SUB(K,3)
    343 IF ((LINE.NE.10) .AND. K.NE.NS) GO TO 350
    IF (LINE.EQ.6) GO TO 1800
    WRITE(6,345) (Z(LN,1),Z(LN,2),Z(LN,3),LN=1,LINE)
    345 FORMAT (10(1X,3A4))
    LINE= 0
    350 CONTINUE
    IF (.NOT.MOLES) WRITE(6,360)
    360 FORMAT(78HNOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXI
    2DANT IN TOTAL OXIANTS )
    WRITE(6,1100) MOLE
    1100 FORMAT(1H0.*VISCOSITY AND CONDUCTIVITY VALUES BASED ON *.F5.1.* PE
    ARGENT-OF GAS MIXTURE*)
    1000 RETURN
    END

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P1712 01888
 P1712 01889
 P1712 01890
 P1712 01891
 P1712 01892
 P1712 01893
 P1712 01894
 P1712 01895
 P1712 01896
 P1712 01897
 P1712 01898
 P1712 01899
 P1712 01900
 P1712 01901
 P1712 01902
 P1712 01903
 P1712 01904
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 P1712 01909
 P1712 01910
 P1712 01911
 P1712 01912
 P1712 01913
 P1712 01914
 P1712 01915
 P1712 01916
 P1712 01917
 P1712 01918
 P1712 01919
 P1712 01920
 P1712 01921
 P1712 01922
 P1712 01923
 P1712 01924
 P1712 01925
 P1712 01926
 P1712 01927
 P171201 00002
 P171201 00003
 P171201 00004
 P1712 01928
 P1712 01929

```

SUBROUTINE RATIO
C
C      USED FOR AREA RATIO INTERPOLATION ONLY
C
C      DOUBLE PRECISION G,X
C      LOGICAL EQL, FROZ,TPSP
C
C      DIMENSION PER(2,2),AI(13),APCP(13),AT(13),ANMT(13),RP(2),NV(13)
C      1 , RPP(2)
C
C      COMMON/POINTS/NSUM(13),SSUM(13),CPR(13),OLVTP(13),OLVPT(13)
C      1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),MM(13),SONVEL(13),TTT(13)
C      2 ,CTM(13)
C      COMMON/SPECIES/COEF(2,7,150),S(150),EN(150,13),ENLN(150),MO(150)
C      1 ,DELN(150),A(15,150),SUG(150,3),IUSE(150),TEMP(150,2)
C      COMMON/MISC/ENN,SUMN,TY,S9,ATOM(3,101),LLMT(15),BU(15),BOP(15,2)
C      1 ,TM,TLOM,THIO,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,MSUBU,AC(2),AM(2)
C      2 ,HPP(2),RHO(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)
C      3 ,ANMT(13,2),PCMT(13,2),ENTM(13),FAZ(13),RTEMP(13),FOX(15),DENSE(13)
C      4 ,RHOP,KMM(15),TLN,JANF
C      COMMON/DOUBLE/ G(20,21), X(20)
C      COMMON/INDX/ IOLEBUG,CONVG,IP,HP,SP,MPSP,TPSP,MOLES,NP,NT,NPT,L,NS,
C      1 ,MAT,IMAT,IOIN,J,NOMIT,IP,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVELJ
C      2 ,IONS,NC,INSERT,JJSOL,JLIQ,KASE(14),JREAC,IC,IG2
C      COMMON/PCP/PCP(26),VMOCT(13),SPMT(13),YAGI(13),SUBAK(13),SUPAK(13)
C      1 ,CPRF(13),AEAT(13),CSTR,EQL,FROZ,SSO
C      COMMON/OUTP/FMT(30),FP(4),FT(4),FM(4),FS(4),FH(4),FV(4),FO(4)
C      1 ,FC(4),FG(4),FB,FMT(3),F1,F2,F3,F4,F5,FL(4),FMT9,FAL,FA2
C      2 ,FR1,FC1,FN(4),F1(4),FA(4),FI(4),F19X,F0
C
C      EQUIVALENCE (V, NV)
C
C      MBLO = NPT-2
C      DO 22 J=3,NPT
C      IF (PCP(J),GT,PCP(2))GO TO 30
C      22 CONTINUE
C      GO TO 31
C      30 NBLO=J-3
C      31 DO 1200 ISONIC=1,2
C      LL = 1
C      IF (ISONIC.EQ.2) GO TO 34
C      IF (NSUB.EQ.0) GO TO 1200
C      NAR = NSUB
C      GO TO 36
C      34 IF (NSUP.EQ.0) GO TO 1200
C      NAR = NSUP
C      36 DO 1100 I=1,NAR
C      IF (ISONIC.EQ.2) GO TO 40
C      IF (NBLO.EQ.1) GO TO 1100
C      K=2+NBLO
C      DO 38 JJ=4,K
C      J=JJ
C      V(LL) = SUBAR(I)

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SUBROUTINE	NAME	FORTRAN EXTENDED VERSION 2.0	31/12/70	08.09.56.	PAGE NO. 2
55	IFV(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*NSLO			P1712 01788	
60	DO 42 JJ=K,NPT			P1712 01789	
	J=JJ			P1712 01790	
	IF(V(LL),LE,AEAT(J)) GO TO 56			P1712 01791	
-2	CONTINUE			P1712 01792	
	IF(V(LL),GE,AEAT(J)*3.) GO TO 85			P1712 01793	
65	56 KJ = J-1			P1712 01794	
	K = KJ			P1712 01795	
	DO 64 JJ=1,2			P1712 01796	
	IF(OPR(K).NE.0.) GO TO 63			P1712 01797	
	WRITE(6,62)K			P1712 01798	
70	62 FORMAT(17H0CANNOT USE POINT,12,3X,4HCP=0)			P1712 01799	
	GO TO 1100			P1712 01800	
61	PER(JJ,II)=1.7CPR(K)*WM(K)			P1712 01801	
	IF (EQL) PER(JJ,1) = PER(JJ,1)*DLVTP(K)			P1712 01802	
75	PER(JJ,2) = TTT(K)/E.*WM(K)*(HSUM(1)-HSUM(K))			P1712 01803	
	RP(JJ) = 1./(1./GAMMA(K)-PER(JJ,2))			P1712 01804	
	IF(EQL)RPP(JJ) = 1.*DLVTP(K)+(1.-DLVTP(K))*PER(JJ,1)			P1712 01805	
	K = KJ + 1			P1712 01806	
66	CONTINUE			P1712 01807	
75	AMAT(LL) = WM(1)			P1712 01808	
80	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),AMNT(LL))			P1712 01811	
	K = KJ			P1712 01812	
85	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.-GAMMA(K))/GAMMA(K)*G(JJ+2,7)			P1712 01816	
	G(JJ,1)=1.			P1712 01817	
	G(JJ+2,1)=0			P1712 01818	
90	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 P=3,5			P1712 01823	
95	MXG=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	
100	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	
76	CONTINUE			P1712 01831	
	INAT = 6			P1712 01832	
105	CALL MGAUSS			P1712 01833	
	AI(LL) = X (1)			P1712 01834	
	DO 84 JJ=2,6			P1712 01835	

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SUBROUTINE RATIO FORTAN EXTENDED VERSION 2.0

Line	Code	Statement	Address
160	C	G*	P1712 01889
	C		P1712 01890
	C		P1712 01891
	C	FMT(5)=FMT(9	P1712 01892
	C	00 94 M=1,LL	P1712 01893
165	C	NV(M)=CSTR+.5	P1712 01894
	C	94 CONTINUE	P1712 01895
	C	WRITE(6,FMT) (FR(M),N=1,4), (NV(M),M=1,LL)	P1712 01896
	C		P1712 01897
	C	CF - IMRUST COEFFICIENT	P1712 01898
170	C		P1712 01899
	C	00 95 M=1,LL	P1712 01900
	C	V(FR(M)*32.174/CSTR	P1712 01901
	C	95 CONTINUE	P1712 01902
	C	FMT(5)=F8	P1712 01903
	C	FMT(7)=F3	P1712 01904
175	C	WRITE(6,FMT) FC1,F8,F8,F8,(VIN),M=1,LL)	P1712 01905
	C	WRITE(6,96)	P1712 01906
	C	96 FORMAT(')	P1712 01907
	C		P1712 01908
180	C	PRESSURE RATIO	P1712 01909
	C		P1712 01910
	C	FMT(4)=FMT(6)	P1712 01911
	C	00 97 M=1,LL	P1712 01912
	C	K=2*M+3	P1712 01913
185	C	FMT(K)=F3	P1712 01914
	C	IF(APCP(M).GE.1000.) FMT(K)=F2	P1712 01915
	C	IF(APCP(M).GE.10000.) FMT(K)=F1	P1712 01916
	C	97 CONTINUE	P1712 01917
	C		P1712 01918
190	C	PRESSURE	P1712 01919
	C		P1712 01920
	C	WRITE(6,FMT) FR1,F8,F8,F8,(APCP(M),M=1,LL)	P1712 01921
	C	00 98 M=1,LL	P1712 01922
	C	K=2*M+3	P1712 01923
195	C	V(M)=P(1)/APCP(M)	P1712 01924
	C	FMT(K)=F3	P1712 01925
	C	IF(VIN).GE.1.) FMT(K)=F3	P1712 01926
	C	IF(VIN).GE.10.) FMT(K)=F2	P1712 01927
	C	IF(VIN).GE.100.) FMT(K)=F1	P1712 01928
200	C	98 CONTINUE	P1712 01929
	C	WRITE(6,FMT) (FFIN),N=1,4), (V(M),M=1,LL)	P1712 01930
	C		P1712 01931
	C	TEMPERATURE	P1712 01932
	C		P1712 01933
205	C	00 101 M=1,LL	P1712 01934
	C	NV(M)=AT(M)+.5	P1712 01935
	C	101 CONTINUE	P1712 01936
	C	FMT(4)=FMT(9	P1712 01937
	C	FMT(5)=FMT(9	P1712 01938
210	C	WRITE(6,FMT) (FT(N),N=1,4), (NV(M),M=1,LL)	P1712 01940
	C		P1712 01941
	C	ENTHALPY	P1712 01941

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SUBROUTINE RATIO FORTRAN EXTENDED VERSION 2.0

```

C
      FMT(5)=F8
      FMT(7)=F1
      DO 104, M=1,LL
      V(M)=MSUM(1)*R-1000.*(AI(M)/294.38)**2
104 CONTINUE
      WRITE(6,FMT) (P(M),M=1,N), (V(M),M=1,LL)
C
220  C      ENITROPY
C
      FMT(7)=F4
      V(1)=SSUM(2)*R
      DO 106, M=1,LL
      V(M)=V(1)
106 CONTINUE
      WRITE(6,FMT) (FS(M),M=1,4), (V(M),M=1,LL)
C
230  C      MOLECULAR HEIGHT
C
      FMT(7)=F3
      WRITE(6,FMT) (FM(M),M=1,4), (AMT(M),M=1,LL)
110 CONTINUE
120 CONTINUE
      RETURN
      END

```

```

SUBROUTINE REACT
C
C
C DOUBLE PRECISION G,X
C LOGICAL HP,SP,TP,IOEBUG,CONVG,NEMR,IONS,MOLES,EOL,FROZ
C DIMENSION NAME(12),V(12)
C
COMMON/HISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),80(15),80P(15,2)
1  * TM,TLCH,TMID,THIGH,PP,CPSON,OF,EQAT,FCPT,R,RR,HSUB8,AC(2),AK(2)
2  * HPP(2),RHO(2),VWIN(2),VPLS(2),MPI(2),DATA(22),NAME(15,5)
3  * ANUM(15,5),PECHT(15),ENTH(15),FAZ(15),RTMP(15),FOX(15),DENS(15)
4  * HOP,CHM(15),TEN,JANE
COMMON/INDX/ IOEBUG,CONVG,IP,HP,SP,HPSP,TPSP,MOLES,NP,NT,NPT,L,NS,
15 1  KMAT,IMAT,IG1,N,J,NOHIT,IP,NEMR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2  * IONS,NC,NSERT,JSOL,JLIQ,KASE(14),NREAC,IG,IQ2
C EQUIVALENCE (NAME,ANAME)
C
20 DATA MOL/1HM/,OX/1HO/,LANK/1M /,IZERO/2H00/
C
WRITE(6,3000)
9000 FORMAT(1M,'*REACTANTS*')
DO 10 K=1,2
  NP(K)=0
  HPP(K)=0
  RHC(K)=0
  VPLS(K)=0
  VWIN(K)=0
  AC(K)=0
  AN(K)=0
  DO 8 J=1,15
    LLMT(J)=0
    BOP(J,K)=0
  8 CONTINUE
  10 CONTINUE
  N=1
  L=1
  NREACS=NREAC
  IF (NREAC.GT.16) NREAC=16
  DO 200 N=1,NREAC
    20 READ(5,21) (NAME(N,I),ANUM(N,I),I=1,5),PECHT(N),MOLE,ENTH(N),FAZ(N)
    1  * RTMP(N),FOX(N),DENS(N)
    21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F8.5,A1,F8.5)
    IF (L.EQ.0) GO TO 20
    IF (NAME(N,1).EQ.LANK) GO TO 200
    WRITE (6,31) (NAME(N,I),ANUM(N,I),I=1,5),PECHT(N),MOLE,ENTH(N),FAZ
    1  (N),RTMP(N),FOX(N),DENS(N)
    31 FORMAT(1X,5(A2,1X,F7.5),F7.5,2X,1X,F9.5,2X,1X,F8.5,2X,1X,F8.5,2X,
    1A1,3X,F8.5)
    50 IF (MOLE.EQ.MOL) MOLES=.TRUE.
    K=2
    IF (FOX(N).EQ.OX) K=1

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SUBROUTINE REACT FORTRAN EXTENDED VERSION 2.0

```
55      DO 38 J=1,15
          DATA(J) = 0.
          38 CONTINUE
          RM=0.
          GO 100 JJ=1,5
          IF (ANUM(N,JJ).EQ.0.) GO TO 101
          DO 41 J=1,15
              NJ = J
              IF (LLMT(J).EQ.0) GO TO 45
              IF (NAME(N,JJ).EQ.LLMT(J)) GO TO 46
              41 CONTINUE
              45 L = NJ
              LLPT(J)=NAME(N,JJ)
              46 DO 48 KK=1,101
                  IF (ATOM(1,KK).EQ.ANAME(N,JJ)) GO TO 50
                  48 CONTINUE
                  L=0
                  GO TO 20
              50 RM=RM+AMU(N,JJ)*ATOM(2,KK)
                  V(J)=ATOM(3,KK)
                  DATA(J)=ANUM(N,JJ)
              100 CONTINUE
              101 PCMT=PECHT(N)
                  IF (MOLES) PCMT=PCMT*RM
                  MP(NT=MP(T)+PCMT
                  IF (NAME(N,5).NE.1ZER0) HPP(K)=HPP(K)+ENTH(N)*PCMT/RM
                  AM(K)=AM(K)+PCMT/R4
                  DO 110 J=1,L
                      80 F(J,K)=DATA(J)*PCMT/RM +90P(J,K)
                      110 CONTINUE
                  IF (DENSE*NE.0.) GO TO 115
                      GO TO 117
                  115 RHQ(K)=RHQ(K)+PCMT/DENS(N)
                  117 RMK(N) = RM
                  200 CONTINUE
                  IF (NREAGS.LE.16) GO TO 1205
                      NRAM=NREAGS-16
                      DO 1200 I=1,NRAM
                          1200 READ(15,21) JUNK
                          1205 IF (L.EQ.0) GO TO 1000
                              IF (L.EQ.0) GO TO 1000
                              DO 220 K=1,2
                                  IF (MP(K).EQ.0.) GO TO 220
                                  HPP(K)=HPP(K)/MF(K)
                                  AM(K) = MP(K)/AM(K)
                                  IF (RHO(K).NE.0.) RHQ(K)=MP(K)/RHO(K)
                                  DO 215 J=1,L
                                      80 P(J,K)=80P(J,K)/MP(K)
                                  IF (V(J).GT.0.) VPM(K)=VPM(K)+80P(J,K)*V(J)
                                  IF (V(L).GT.0.) VPLS(K)=VPLS(K)+80P(J,K)*V(J)
                                  215 CONTINUE
                                  IF (MOLES) GO TO 220
                                  DO 216 N=1,NREAL
```

SUBROUTINE REACT		FORTRAN EXTENDED VERSION 2.0		31/12/70	06:09:56	PAGE NO. 3
110	IF (FOX(N) = 0.0X.AND.N.EQ.2) GO TO 218	P1712	02073			
	IF (FOX(N) .NE. 0X.AND. L.EQ.1) GO TO 218	P1712	02074			
	PECMT(N) = PECMT(N)/WP(K)	P1712	02075			
	218 CONTINUE	P1712	02076			
	220 CONTINUE	P1712	02077			
	NEWR = TRUE.	P1712	02078			
	DO 230 N = 1,NREAC	P1712	02079			
	IF (DENS(N) .NE. C.) GO TO 230	P1712	02080			
115	RHC (1) = 0.	P1712	02081			
	GO TO 1800	P1712	02082			
	230 CONTINUE	P1712	02083			
	1000 RETURN	P1712	02084			
	END	P1712	02085			

SUBROUTINE RKTOU1		
C	ROCKET PERFORMANCE PARAMETERS	P1712 02086
C		P1712 02087
C		P1712 02088
C		P1712 02089
C		P1712 02090
C		P1712 02091
C	LOGICAL EQL,FROZ ,TP,HP,SP,HPSP,TPSP,SHOCK	P1712 02092
C		P1712 02093
C		P1712 02094
C		P1712 02095
C		P1712 02096
C		P1712 02097
C		P1712 02098
C		P1712 02099
C		P1712 02100
C		P1712 02101
C		P1712 02102
C		P1712 02103
C		P1712 02104
C		P1712 02105
C		P1712 02106
C		P1712 02107
C		P1712 02108
C		P1712 02109
C		P1712 02110
C		P1712 02111
C		P1712 02112
C		P1712 02113
C		P1712 02114
C		P1712 02115
C		P1712 02116
C		P1712 02117
C		P1712 02118
C		P1712 02119
C		P1712 02120
C		P1712 02121
C		P1712 02122
C		P1712 02123
C		P1712 02124
C		P1712 02125
C		P1712 02126
C		P1712 02127
C		P1712 02128
C		P1712 02129
C		P1712 02130
C		P1712 02131
C		P1712 02132
C		P1712 02133
C		P1712 02134
C		P1712 02135
C		P1712 02136
C		P1712 02137
C		P1712 02138

55	C	PRESSURE RATIOS	P1712 02139
	C		P1712 02140
	C	DO 45 I=1,NPT	P1712 02141
	C	K=2*I+3	P1712 02142
	C	FMT(K)=F3	P1712 02143
	C	IF (PCP(I).GE.1000.) FMT(K)=F2	P1712 02144
	C	IF (PCP(I).GE.1000.) FMT(K)=F1	P1712 02145
	C	IF (PCP(I).GE.10000.) FMT(K)=F1	P1712 02146
	C	IF (PCP(I).GE.100000.) FMT(K)=F1	P1712 02147
	C	IF (PCP(I).GE.1000000.) FMT(K)=F1	P1712 02148
	C	IF (PCP(I).GE.10000000.) FMT(K)=F1	P1712 02149
	C	IF (PCP(I).GE.100000000.) FMT(K)=F1	P1712 02150
	C	IF (PCP(I).GE.1000000000.) FMT(K)=F1	P1712 02151
	C	IF (PCP(I).GE.10000000000.) FMT(K)=F1	P1712 02152
	C	IF (PCP(I).GE.100000000000.) FMT(K)=F1	P1712 02153
	C	IF (PCP(I).GE.1000000000000.) FMT(K)=F1	P1712 02154
	C	IF (PCP(I).GE.10000000000000.) FMT(K)=F1	P1712 02155
	C	IF (PCP(I).GE.100000000000000.) FMT(K)=F1	P1712 02156
	C	IF (PCP(I).GE.1000000000000000.) FMT(K)=F1	P1712 02157
	C	IF (PCP(I).GE.10000000000000000.) FMT(K)=F1	P1712 02158
	C	IF (PCP(I).GE.100000000000000000.) FMT(K)=F1	P1712 02159
	C	IF (PCP(I).GE.1000000000000000000.) FMT(K)=F1	P1712 02160
	C	IF (PCP(I).GE.10000000000000000000.) FMT(K)=F1	P1712 02161
	C	IF (PCP(I).GE.100000000000000000000.) FMT(K)=F1	P1712 02162
	C	IF (PCP(I).GE.1000000000000000000000.) FMT(K)=F1	P1712 02163
	C	IF (PCP(I).GE.10000000000000000000000.) FMT(K)=F1	P1712 02164
	C	IF (PCP(I).GE.100000000000000000000000.) FMT(K)=F1	P1712 02165
	C	IF (PCP(I).GE.1000000000000000000000000.) FMT(K)=F1	P1712 02166
	C	IF (PCP(I).GE.10000000000000000000000000.) FMT(K)=F1	P1712 02167
	C	IF (PCP(I).GE.100000000000000000000000000.) FMT(K)=F1	P1712 02168
	C	IF (PCP(I).GE.1000000000000000000000000000.) FMT(K)=F1	P1712 02169
	C	IF (PCP(I).GE.10000000000000000000000000000.) FMT(K)=F1	P1712 02170
	C	IF (PCP(I).GE.100000000000000000000000000000.) FMT(K)=F1	P1712 02171
	C	IF (PCP(I).GE.1000000000000000000000000000000.) FMT(K)=F1	P1712 02172
	C	IF (PCP(I).GE.10000000000000000000000000000000.) FMT(K)=F1	P1712 02173
	C	IF (PCP(I).GE.100000000000000000000000000000000.) FMT(K)=F1	P1712 02174
	C	IF (PCP(I).GE.1000000000000000000000000000000000.) FMT(K)=F1	P1712 02175
	C	IF (PCP(I).GE.10000000000000000000000000000000000.) FMT(K)=F1	P1712 02176
	C	IF (PCP(I).GE.100000000000000000000000000000000000.) FMT(K)=F1	P1712 02177
	C	IF (PCP(I).GE.1000000000000000000000000000000000000.) FMT(K)=F1	P1712 02178
	C	IF (PCP(I).GE.10000000000000000000000000000000000000.) FMT(K)=F1	P1712 02179
	C	IF (PCP(I).GE.100000000000000000000000000000000000000.) FMT(K)=F1	P1712 02180
	C	IF (PCP(I).GE.1000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02181
	C	IF (PCP(I).GE.10000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02182
	C	IF (PCP(I).GE.100000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02183
	C	IF (PCP(I).GE.1000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02184
	C	IF (PCP(I).GE.10000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02185
	C	IF (PCP(I).GE.100000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02186
	C	IF (PCP(I).GE.1000000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02187
	C	IF (PCP(I).GE.10000000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02188
	C	IF (PCP(I).GE.100000000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02189
	C	IF (PCP(I).GE.1000000000000000000000000000000000000000000000000.) FMT(K)=F1	P1712 02190

110	C	FMT(4) = FMT9X FMT(5) = FMT13 FMT(6) = FMT19 FMT(7) = F3 WRITE(6,FMT)(FR(I),I=1,4),(NV(J),J=2,NPT)	P1712 02191 P1712 02192 P1712 02193 P1712 02194 P1712 02195 P1712 02196 P1712 02197
115	C	CF = THPST COEFFICIENT FMT(6) = FMT(8) FMT(7) = F3 DO 212 I=2,NPT	P1712 02198 P1712 02199 P1712 02200 P1712 02201 P1712 02202
120	C	212 V(I)=32.174*SPIK(I)/CSTR WRITE(6,FMT)FC1,FB,FB,FB,(V(J),J=2,NPT)	P1712 02203 P1712 02204 P1712 02205 P1712 02206 P1712 02207 P1712 02208
125	C	AREA RATIO FMT(5) = F3 DO 214 I = 2,NPT K = 2*1+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	P1712 02209 P1712 02210 P1712 02211 P1712 02212 P1712 02213 P1712 02214 P1712 02215 P1712 02216 P1712 02217 P1712 02218 P1712 02219 P1712 02220
130	C	214 CONTINUE WRITE(6,FMT)FA1,FA2,FB,FB,(AEAT(J),J=2,NPT)	P1712 02221 P1712 02222 P1712 02223 P1712 02224 P1712 02225 P1712 02226
135	C	VACUUM IMPULSE FMT(5) = FMT13 FMT(7) = F1 WRITE(6,FMT)(FA(I),I=1,4),(VAGI(J),J=2,NPT)	P1712 02227 P1712 02228 P1712 02229 P1712 02230 P1712 02231 P1712 02232
140	C	SPECIFIC IMPULSE WRITE(6,FMT)(F1,I=1,4),(SPIM(J),J=2,NPT)	P1712 02233 P1712 02234 P1712 02235 P1712 02236 P1712 02237 P1712 02238
145	C	WRITE(6,208) FMT(4) = F3 FMT(5) = FMT13 FMT(7) = F5 IF(COL) GO TO 312 WRITE(6,310)	P1712 02239 P1712 02240 P1712 02241 P1712 02242 P1712 02243
150	C	310 FORMAT(15H0MOLE FRACTIONS //)	
155	C	MOLE FRACTIONS - FROZEN LINE = 0 DO 431 K=1,MS V(LINE+1) = EN(K,1)/TOTN(1) IF (V(LINE+1).LT.(9.E-6)) GO TO 424 LINE = LINE+1 24LINE,1) = SUB(K,1)	

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160	Z(LINE,2) = 3(K,2) Z(LINE,3) = SUB(K,3) Z(LINE,4) = V(LINE)		P1712 02244 P1712 02245 P1712 02246	
424	IF (LINE.NE.4.AND.K.NE.NS) GO TO 430 IF (LINE.EQ.0) GO TO 312 WRITE (6,426) (Z(LN,1),Z(LN,2),Z(LN,3),Z(LN,4),LN=1,LINE)		P1712 02247 P1712 02248 P1712 02249	
165	426 FORMAT (1H,4TSAN,9.5,7X) LINE = 0		P1712 02250 P1712 02251	
	430 CONTINUE		P1712 02252	
	712 CALL OUT3		P1712 02253	
170	1000 RETURN END		P1712 02254 P1712 02255	

		P1712	02256
C	SUBROUTINE ROCKET	P1712	02256
C		P1712	02257
C	ROCKET PERFORMANCE	P1712	02258
C	EITHER HPSP OR TPSP IS TRUE	P1712	02259
C		P1712	02260
C		P1712	02261
C	LUGICAL HP, SP, TP, TUEBUG, NEWB, IONS, NOLESJ, FROZ, EOL, LOGV, HPSP, TPSP	P1712	02262
C		P1712	02263
C	DIMENSION AA(2), BB(2), CC(2)	P1712	02264
C		P1712	02265
C	COMMON/POINTS/HSEUH(13), SSUM(13), CPR(13), DLVTP(13), DLVPT(13)	P1712	02266
C	1. GAMMAS(13), P(26), T(26), V(13), PPP(13), HH(13), SONVEL(13), TTT(13)	P1712	02267
C	2. TCNTN(13)	P1712	02268
C	COMMON/SPECES/CDEF(2,7,150), S(150), EN(150,13), ENLN(150), HQ(150)	P1712	02269
C	1. CELN(150), A(15,150), SUB(150,3), IUSE(150), TEMP(50,2)	P1712	02270
C	COMMON/ATSC/ENN, SUMN, TT, SU, ATOM(3,101), LLMT(15), BOP(15,2)	P1712	02271
C	1. TN, FLOW, THIO, THIGH, PP, CPSUM, OF, EGRTAT, PCPT, R, RR, HSUBO, ACI(2), AH(2)	P1712	02272
C	2. HPP(2), RHOD(2), VMIN(2), VPLS(2), WP(2), DATA(22), NAME(15,5)	P1712	02273
C	3. ANORT(15,5), PECHT(15), ENTH(15), FAZ(15), XTEMP(15), FOX(15), DENSI(15)	P1712	02274
C	4. RHOP, RNW(15), TLN, JANF	P1712	02275
C	COMMON/INDX/ IDEBUS, CONVG, TP, HP, SP, HPSP, I' SP, NOLES.NP, NT, NPT, L, NS,	P1712	02276
C	1. KMAT, TMAT, IQI, N, J, NOMIT, IP, NEWR, NSUB, NSUP, ITN, CPCVFR, CPQVEO	P1712	02277
C	2. IONS, NC, NSERT, JSOL, JLIO, KASE(14), NREAC, IC, IO2	P1712	02278
C	COMMON/PERF/PCP(26), VHOC(13), SPIH(13), VAGI(13), SUBAR(13), SUPAR(13)	P1712	02279
C	1. CUPR(13), KEAT(13), CSTK, EGL, FROZ, SSU	P1712	02280
C	COMMON/CVOLUN/ VOLUNC, IMPETUS, IFLG6G	P1712	02281
C	REAL IMPETUS	P1712	02282
C		P1712	02283
C	NAPELIST/RKTNP/EOL, FROZ, SUBAR, SUPAR, PCP	P1712	02284
C		P1712	02285
C	ITM = 0	P1712	02286
C	IFLG6G=0	P1712	02287
C	210 DO 300 I=1,26	P1712	02288
C	PCP(I)= 0.	P1712	02289
C	SUZAR(I) = 0.	P1712	02290
C	300 CONTINUE	P1712	02291
C	HPSP = .TRUE.	P1712	02292
C	HP = .TRUE.	P1712	02293
C	TPSP = .FALSE.	P1712	02294
C	EOL = .TRUE.	P1712	02295
C	FRCZ = .TRUE.	P1712	02296
C	READ (5,RKTNP)	P1712	02297
C	IF (TTT.CO.GT.) GO TO 302	P1712	02298
C	TPSP = .TRUE.	P1712	02299
C	TP = .TRUE.	P1712	02300
C	HPSP = .FALSE.	P1712	02301
C	GO TO 303	P1712	02302
C	302 T(1) = 3800.	P1712	02303
C	303 IF (PCP(1).NE.0.) GO TO 308	P1712	02304
C	DO 305 I=1,NP	P1712	02305
C	K = NP-1+I	P1712	02306
C	P(K) = P(K-1)	P1712	02307
C	308 CONTINUE	P1712	02308

Line	Code	Statement	Label
55		GO TO 311	P1712 02309
59A	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
60		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
65		DO 320 I=1,13	P1712 02320
		IF (SUBART(I).NE.0.) NSUB=NSUB+1	P1712 02321
		IF (SUPART(I).NE.0.) NSUP=NSUP+1	P1712 02322
320	CONTINUE		P1712 02323
		WRITE (6,RTINP)	P1712 02324
70		SS0 = 0.	P1712 02325
		ITROT = 3	P1712 02326
		IT = 1	P1712 02327
	C		P1712 02328
	C	SET ASSIGNED P	P1712 02329
75			P1712 02330
		DO 902 IP = 1, NP	P1712 02331
		PP = P(IP)	P1712 02332
		CALL ECDROM	P1712 02333
		T(NPT) = IT	P1712 02334
90		IF (IT.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
87		IF (IP.GT.1) GO TO 199	P1712 02339
85			P1712 02340
	C		P1712 02341
	C	COMBUSTION CHAMBER	P1712 02342
		IP = .FALSE.	P1712 02343
90		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
		IT = 2 * IT / (GAMMAS(1)+1.)	P1712 02349
95		GO TO 900	P1712 02350
199		IF (IP.GT.2) GO TO 900	P1712 02351
	C		P1712 02352
	C	THROAT	P1712 02353
100		IF (ITH.NE.2) GO TO 191	P1712 02354
		ITH = 0	P1712 02355
		GAMMAS(2) = 0.	P1712 02356
		GO TO 900	P1712 02357
191		OH = HSUM(1)-HSUM(2)	P1712 02358
105		DHSTAR = OH-GAMMAS(2) * IT * ENN / 2.	P1712 02359
		IF (IDEPUG) WRITE (6,923) DHSTAR, HSUM(1), HSUM(2), PCP(2)	P1712 02360
			P1712 02361

923 FORMAT(4E25.8)

CH = OMSTAR/DM

IF (DM.LT.0.) OH=OH

IF (DM.LT.0.4E-04) IFROT.EQ.0) GO TO 900

IF (JSOL.NE.0) ITH = 1

IF (JSOL.EQ.0) ITH=2

IF (ITH.EQ.0) GO TO 192

C SPECIAL THROAT INTERPOLATION IF ITH = 2

C

C

DLNI = .5*TT*ENN/(HSUM(1)-HSUM(2))

AA(ITH) = .5*DLNI*(2.*DLNI*(54*MAS(2)-1.)/GAMMAS(2))

XX = ALOG(PCP(2))

98(ITH) = 1./GAMMAS(2)-DLNI-2.*XX*AA(ITH)

GC(ITH) = ENW*TT/(PP*(HSUM(1)-HSUM(2))*0.5)

CC(ITH) = ALOG(CC(ITH))-XX*(38(ITH)+AA(ITH)*XX)

IF (ITH.EQ.1) GO TO 192

DB(1)=8E(1)-88(2)

TATY=XX*(1)-AT(2)

PCP(2)=(-39(1)+(88(1)*88(1)-4.*AA(1)*(CC(1)-CC(2))*0.5)/(2.*AA(1))

1) PCP(3)=EXP(PCP(2))

GO TO 193

192 PCP(2) = PCP(2)/(1.+2.*DHSTAR/(ENN*TT*(GAMMAS(2)+1.)))

193 P(2) = P(1) / PCP(2)

PP = P(2)

IFROT = ITROT-1

CALL EOLBRN

IF (TT.EQ.0.) GO TO 1000

GO TO 190

88

C 900 K = 0

IF (.NOT.EQ. .AND. FROZ) GO TO 990

IF (IP.EQ.NP.OR.TT.EQ.0.) GO TO 860

K = NPT

IF (NPT.NE.13) GO TO 870

860 CALL RK70T

IFLGG=1

IF ((NSUB + NSUP).NE.0) CALL RATIO

IF (K.EQ.0) GO TO 930

WRITE(6,865)

865 FORMAT(1H1)

NPT = 2

870 NPT = NPT + 1

C SAVE COMPOSITIONS FOR ESTIMATES OF NEXT POINT

C

DO 880 I = 1,NS

ENTINPT) = ENTIN(K)

880 CONTINUE

902 CONTINUE

990 IF (FROZ) CALL FROZEN

1000 RETURN

P1712 02362

P1712 02363

P1712 02364

P1712 02365

P1712 02366

P1712 02367

P1712 02368

P1712 02369

P1712 02370

P1712 02371

P1712 02372

P1712 02373

P1712 02374

P1712 02375

P1712 02376

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P1712 02378

P1712 02379

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P1712 02381

P1712 02382

P1712 02383

P1712 02384

P1712 02385

P1712 02386

P1712 02387

P1712 02388

P1712 02389

P1712 02390

P1712 02391

P1712 02392

P1712 02393

P1712 02394

P1712 02395

P1712 02396

P1712 02397

P1712 02398

P1712 02399

P1712 02400

P1712 02401

P1712 02402

P1712 02403

P1712 02404

P1712 02405

P1712 02406

P1712 02407

P1712 02408

P1712 02409

P1712 02410

P1712 02411

P1712 02412

P1712 02413

P1712 02414

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160 ~~END~~ ~~P1712~~ ~~02419~~

		SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED		
05	C	INTEGER SUB, OMIT, ENL	P1712	02416
	C	LOGICAL NEWB	P1712	02417
	C		P1712	02418
	C		P1712	02419
	C		P1712	02420
	C		P1712	02421
	C		P1712	02422
10	C	DIMENSION DATE(2,3), HT(4), B(4), OMIT(3,3)	P1712	02423
	C	COMMON/SPECIES/CDEF(2,7,150), EN(150,13), ENLN(150), MO(150)	P1712	02424
	C	1, CELN(150), A(15,150), SUB(150,3), IUSE(150), TEMPI(50,2)	P1712	02425
	C	COMMON/MISC/ENN, SUMN, TT, SU, ATOM(13,101), LLMT(15), B0(15), B0P(15,2)	P1712	02426
	C	1, TW, TLM, TMC, THIGH, PP, CP, SD, OF, EORAT, FPCT, R, RR, MSUB, AC(2), AM(2)	P1712	02427
	C	2, MP(12), RMO(2), WYIN(2), VPUS(2), WMP(2), DATA(22), NAME(15,5)	P1712	02428
	C	3, ANUM(15,5), PECONT(15), ENTH(15), FAZ(15), RTEMP(15), FOX(15), DEN(15)	P1712	02429
	C	4, QHOP, RMM(15), TLN, JANF	P1712	02430
	C	COMMON/INDEX/ IDEBUG, CONVG, TP, HP, SP, HPS, TPSP, MOLES, NP, NT, WPT, L, NS,	P1712	02431
	C	1, KMAT, IMAT, IOI, N, J, NOMIT, IP, NEWB, NSUB, NSUP, ITR, CPCVFR, CPCVLO	P1712	02432
	C	2, IONS, FC, NSERT, JSOL, JULIO, KASE(147), NREAC, IC, IOZ	P1712	02433
20	C	EQUIVALENCE (DATE, EN), (OMIT, ENLN), (END, END)	P1712	02434
	C	DATA GAS/ING/, END/3END/	P1712	02435
	C		P1712	02436
	C		P1712	02437
	C		P1712	02438
	C		P1712	02439
25	C	NC=0	P1712	02440
	C	IX=0	P1712	02441
	C	COEF(1,1,1) = ENDD	P1712	02442
	C	DC 3 I=1,150	P1712	02443
	C	ISAVE=I	P1712	02444
	C	IF(A(I), I, EQ, ENDD) GO TO 4	P1712	02445
30	C	DO 3 J=1, L	P1712	02446
	C	A(J, I) = 0.	P1712	02447
	C	3 CONTINUE	P1712	02448
	C	4 MAXNS=ISAVE	P1712	02449
	C	REIND 9	P1712	02450
	C	READ (9,5) TLOW, TMID, THIGH	P1712	02451
	C	5 FORMAT (3F10,3)	P1712	02452
	C	NS = 1	P1712	02453
	C	7 READ (9,10) (SUB(NS, I), I=1,3), DATE(1, NS), DATE(2, NS), (HT(J), B(J),	P1712	02454
	C	1 J=1,4), PHAZ, F1, T2	P1712	02455
	C	10 FORMAT (3A4, 5X, 2A3, 3A2, F3, 3), A1, 2F10, 3)	P1712	02456
	C	IF (SUB(NS, I), EQ, ENDD) GO TO 171	P1712	02457
	C	READ (9,20) (COEF(I, J), J=1, 7), I=1, 2)	P1712	02458
	C	20 FORMAT (5E15, 8)	P1712	02459
	C	IF (NOMIT, EQ, 0) GO TO 810	P1712	02460
	C	DC 805 I=1, NOMIT	P1712	02461
	C	DO 804 J=1, 3	P1712	02462
	C	IF (OMIT(J, I), NE, SUB(NS, J)) GO TO 805	P1712	02463
	C	804 CONTINUE	P1712	02464
	C	GO TO 7	P1712	02465
	C	805 CONTINUE	P1712	02466
	C	810 DO 820 K=1, 4	P1712	02467
	C	IF (B(K), EQ, 0) GO TO 825	P1712	02468

```

55      DO 168 I=1,L
          IF (LLMT(I).EQ.MT(K)) GO TO 820
          168 CONTINUE
          DO 819 J=1,L
              819 A(I,J,NS) = 0.
              GO TO 7
          820 A(I,NS) = 819
          825 IF (NS.EQ.HAXNS) GO TO 870
              IUSE(NS) = 0
              IF (PHAZ.EQ.GAS) GO TO 170
              NC = NC+1
              TEMP(NC,1) = T1
              TEMP(NC,2) = T2
              IX = IX+1
              IF (IUSE(NS-1).EQ.0 .OR. NC.EQ.1) GO TO 145
              DO 830 I=1,L
                  830 CONTINUE
                  IF (A(I,NS).NE.A(I,NS-1)) GO TO 145
                  IX = IX+1
                  145 IUSE(NS) = -IX
                  170 NS = NS+1
                  GO TO 7
              870 WRITE(6,871) (SUB(NS,J),J=1,3)
                  871 FORMAT (45H0DIMENSIONS IN/SPECIES/100 SHALL TO CONSIDER ,3A4)
                  GO TO 7
              171 NS = NS-1
                  NEWR = .FALSE.
                  WRITE(6,172)
                  172 FORMAT (42H0SPECIES BEING CONSIDERED IN THIS SYSTEM )
                  DO 174 I=1,NS,5
                      174 IF (NS.LT.I5) I5=NS
                          174 WRITE (6,176) (DATE(1,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I,
                              1 I5)
                          176 FORMAT (5(5X,2A3,2X,3A4))
                          RETURN
                  END
          90

```

P1712 02469

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P1712 02500

P1712 02501

P1712 02502

P1712 02503

P1712 02504

P1712 02505

08.09.56.

31/12/70

FORTHAN EXTENDED VERSION 2.0

SUBROUTINE SET

```

SUBROUTINE SET(ONE,TWO,THREE,ARG,MAL)
C
C      USED FOR AREA RATIO INTERPOLATION ONLY
C      SETS UP ALL 4 BY 5 MATRICES
05  C      DOUBLE PRECISION A,ANS,G,X
C
C      DIMENSION ANS(6),ONE(2),TWO(2),THREE(2),A(20,21)
C
C      COMMON/DOUBLE/G(20,21),X(20)
C      COMMON/INDEX/ IDEBUS,CONVG,TP,HP,SP,HPSP,TPSP,MOLES,MP,NT,NPT,I,LS,
1      KMAT,IMAT,IC1,N,J,NOMIT,IF,NEWR,NSUB,NSUP,ITN,CPCVFR,CPCVEQ
2      IONS,TMO,INSEF,JSOI,JIU,KASE(14),NREAC,IC,IO2
C
C      EQUIVALENCE (G,A),(X,ANS)
C
C      DO 8 J=1,2
A(J,5)=ALOG(ONE(J))
A(J,2)=TWO(J)
A(J,3)=THREE(J)
9 CONTINUE
C      DO 1 I=1,2
A(I,1)=1.0
A(I,2)=0.0
A(I,3)=1.0
10 CONTINUE
C      CALL HGAUSD
MAL=ANS(1)
SUM=ALOG(ARG)
DO 10 J=1,3
MAL=MAL+SUM**J*(ANS(J+1))
10 CONTINUE
MAL=EXP(MAL)
RETURN
END

```

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31/12/78

00.09.56.

PAGE NO. 3

C-----CONDUCTIVITY OF MIXTURE

C

```
110      CONMIX(N)=CONMIX(N)+FMOLE(I)*CONM(I)/SUM
      WRITE(6,9009) VISMIX(M),CONMIX(M),M
      9009 FORMAT(1X,2F15.11,3X,15)
      200 CONTINUE
      1000 CONTINUE
      WRITE(6,2010) (VISMIX(I),I=1,NPT)
      2010 FORMAT(1X,2F15.11,3X,15)
      2000 FORMAT(1H ,*VISC, 5/CM-SEC*,13F9.6)
      2100 FORMAT(1H ,*C, 6AL/6-SEC-K*,13F9.6)
      RETURN
      END
```

P171201 00116
P171201 00117
P171201 00118
P171201 00119
P171201 00120
P171201 00121
P171201 00122
P171201 00123
P171201 00124
P171201 00125
P171201 00126
P171201 00127
P171201 00128

APPENDIX II
POLYNOMIAL FIT PROGRAM

```

PROGRAM SLSCF(INPUT,OUTPUT)
  DIMENSION TT(100),CPR(100),HTR(100),STR(100)
  DIMENSION CCPR(100),CHTR(100),CSTR(100)
  DIMENSION NPT(2),NAME(6)
  COMMON/PATRIX/ G(10,11),X(10),IMAY
  R=1-99726
  ASSIGN 500 TO MEOF
  IF(EOF(MEOF)) 500,500,1
  1 READ 40,MO,NPT,NAME
  40 FORMAT(F10.1,2I3,4X,6A10)
  PRINT 112,NAME,MO
  112 FORMAT('111,29X,6A10//1P',5NH0 = ,F10.1//)
  KPT=0
  111 KPT=KPT+1
  NVAL=NPT(KPT)
  READ 6,(ITT(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.*MO
  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
  SLT=0.
  SLT2=0.
  SLT3=0.
  SLT4=0.
  SLT5=0.
  SLT6=0.
  SLT7=0.
  SLT8=0.
  SLT9=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=T**3
  T4=T**4
  T5=T**5
  T6=T**6
  T7=T**7
  T8=T**8
  T9=T**9
  TREC=1.0/T
  TM2=1.0/T2
  SUMT=SUMT+T

```

15.40.00.

05/01/71

FURTRAN EXTENDED VERSION 2.0

SLSQF

PROGRAM

```

55      SUMT2=SUMT2+T2
      SUMT3=SUMT3+T3
      SUMT4=SUMT4+T4
      SUMT5=SUMT5+T5
      SUMT6=SUMT6+T6
      SUMT7=SUMT7+T7
      SUMT8=SUMT8+T8
60      SUMT2=SUMT2+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
70      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
80      IF(X.GT.1) GO TO 50
      G(1,8)=1.0
      G(1,9)=1.0
      G(1,10)=TLOG
      G(2,6)=FLOAT(INVAL)/2.0
      G(2,8)=T
      G(2,9)=1/2.0
      G(2,10)=1
      G(3,8)=12
      G(3,9)=12/3.
      G(3,10)=1/2.
      G(4,8)=13
      G(4,9)=13/4.
      G(4,10)=13/3.
      G(5,8)=14
      G(5,9)=14/5.
      G(5,10)=1/4.
      G(6,9)=TREC
      G(7,7)=FLOAT(INVAL)
90      G(7,10)=1.0
      G(8,11)=CP
      G(9,11)=HT
      G(10,11)=ST
      50 CONTINUE
      100 CONTINUE
      G(2,2)=G(2,2)+G(1,1)*SUMT2
      G(2,3)=G(2,3)+G(1,3)*SUMT3
      G(2,4)=G(2,4)+G(1,4)*SUMT4
      G(2,5)=G(2,5)+G(1,5)*SUMT5
      G(2,7)=SUMT
      G(3,3)=G(3,3)+G(1,3)*SUMT4
105

```

```

110      G(3,4)=(5./4.)*SUMT5
        G(3,5)=(143./120.)*SUMT6
        G(3,6)=SUMT7/3.
        G(3,7)=SUMT2/2.
        G(4,4)=(169./144.)*SUMT6
        G(4,5)=(117./15.)*SUMT7
        G(4,6)=SUMT2/4.
        G(4,7)=SUMT3/3.
        G(5,5)=(441./400.)*SUMT6
        G(5,6)=SUMT3/5.
        G(5,7)=SUMT4/4.
        G(6,6)=SUMT2
        DO 200 I=1,10
        DC 210 J=1,18
        IF(I.EQ.J) GO TO 213
        G(I,J)=G(I,J)
        210 CONTINUE
        100 CONTINUE
        PRINT 92
        IF(ORIG(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,15E11.5)
        90 CONTINUE
        190 IMAT=10
        CALL HGAUSS
        PRINT 94
        94 FORMAT(1H ,COEFFICIENTS ARE*)
        PRINT 192,X
        192 FORMAT(1X,7E15.8/1X,3E15.8)
        DC 401 I=1,NVAL
        T=TT(I)
        T2=T*T
        T3=T2*T
        T4=T3*T
        T5=T4*T
        T6=T5*T
        T7=T6*T
        T8=T7*T
        T9=T8*T
        T10=T9*T
        TLOG=ALOG(T)
        CCPA(I)=X(1)+X(2)*T+X(3)*T2+X(4)*T3+X(5)*T4
        CCPB(I)=CCPR(I)*R
        CSTR(I)=(X(1)+X(2)*T/2.+X(3)*T2/3.+X(4)*T3/4.+X(5)*T4/5.)*T+X(6)
        100 R
        CSTR(I)=CSTR(I)-H01/1000.
        CSTR(I)=(X(1)+TLOG+X(2)*T+X(3)*T2/2.+X(4)*T3/3.+X(5)*T4/4.)*T+X(7)
        1R
        400 CONTINUE
        PRINT 401
        401 FORMAT(1H , , T CP CCP HT CHT T JST
        1 DCF QMT DST//)
        DO 410 I=1,NVAL
        DCPR=ABS(CPR(I)-CCPR(I))
        DTR=(HT(I)-H01)/1000.
        DMS=ABS(DIR-CMTR(I))
        DSTR=ABS(STR(I)-CSTR(I))

```

PROGRAM	SLSQF	FURTRAN EXTENDED VERSION 2.0	05/01/71	15.40.08.	PAGE NO. 4
160	411	FORMAT(1H,1X,F5.0,9F8.3) PRINT 411,IT(1),CPR(1),CCPR(1),DIR,CHTR(1),STR(1),CSIR(1),DCPR, 1CHTR,OSTR			
165	410	CCTINUE GC 10 (111,1),KPT 500 CONTINUE END			

SUBROUTINE MGAUSD

C SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS

C DOUBLE PRECISION G,X,COEFX(20),SUM,Z
C DIMENSION COEFX(20)

C COMMON/MATRIX/ G(10,10),X(10),IMAT

C EQUIVALENCE (IUSE,IMAT)

C DATA SIGNO/1.E+38/
C DATA SIGNO/1.E+320/

C BEGIN ELIMINATION OF NTH VARIABLE

C IUSE1=IUSE+1

C DO 45 NN=1,IUSE

C IF (NN-IUSE) 8,83,8

C 83 IF (G(NN,NN)) 31,23,31

C SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW

C DO 10 I=NN,IUSE

C COEFX(I) = BIGNO

C IF (G(I,NN).EQ.0.) GO TO 18

C COEFX(I) = 0.

C DO 10 J=NN,IUSE1

C SUM = G(I,J)

C IF (SUM-11.7-1) SUM=-SUM

C IF (J.NE.NN) GO TO 9

C Z = SUM

C GO TO 10

C 9 IF (SUM.GT.COEFX(I)) COEFX(I)=SUM

C 10 CONTINUE

C COEFX(I) = COEFX(I)/Z

C 18 CONTINUE

C TEMP = BIGNC

C I=0

C DO 20 J=NN,IUSE

C IF (COEFX(J)-TEMP) 87,22,22

C 27 TEMP=COEFX(J)

C I=J

C 22 CONTINUE

C IF (I) 20,23,28

C INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH

C VARIABLE FROM THE REMAINING EQUATIONS

C INTERCHANGE EQUATIONS I AND NN

C 28 IF (NN-I) 29,31,29

C 29 DO 30 J=NN,IUSE1

```

55      Z=G(I,J)
      G(I,J)=G(MN,J)
      G(MN,J)=Z
      30 CONTINUE
C
60      C-----DIVIDE MTH ROW BY MTH DIAGONAL ELEMENT AND ELIMINATE THE MTH
      C      VARIABLE FROM THE REMAINING EQUATIONS
      C
      31 K = MN + 1
      DO 36 J = K, IUSE1
      IF((I(MN,MN).EQ.0.) GO TO 23
      G(MN,J) = G(MN,J) / G(MN,MN)
      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,MN)*G(MN,J)
      44 CONTINUE
      45 CONTINUE
C
75      C      BACKSOLVE FOR THE VARIABLES
      C
      47 J = K - 1
      K = IUSE
      X(K) = 0.000
      X(K) = 0.0
      SUM = 0.0
      IF(IUSE = J) 51,48,48
      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
90

```

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